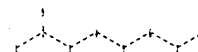
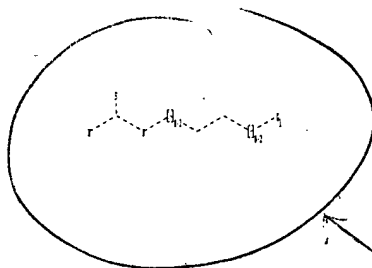


Uploading loe105p.str

HCAPIUS

boxed w/
set of structures
that are
due for
application



chain nodes :
1 2 3 4 7 8 9
ring/chain nodes :
5 6
chain bonds :
1-2 2-3 2-9 3-4 4-5 6-7 7-8
ring/chain bonds :
5-6
exact/norm bonds :
1-2 2-3 2-9 3-4 4-5 5-6 6-7 7-8

G1:O,S,N

Connectivity :

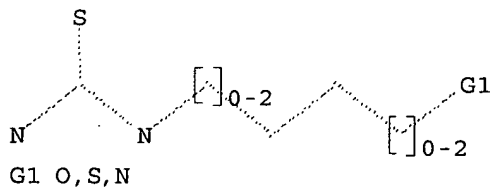
9:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

=> d que stat 16

L4 STR



Structure attributes must be viewed using STN Express query preparation.

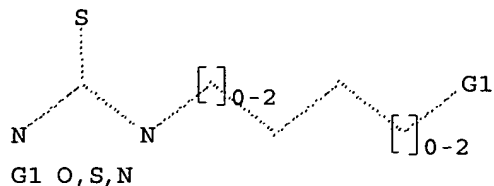
L6 118553 SEA FILE=REGISTRY SSS FUL L4

100.0% PROCESSED 418953 ITERATIONS
SEARCH TIME: 00.00.05

118553 ANSWERS

=> d que stat l25

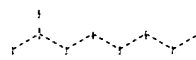
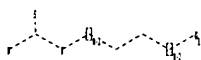
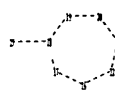
L1 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US2004-840105/APPS
L2 TRANSFER PLU=ON L1 1- RN : 72 TERMS
L3 72 SEA FILE=REGISTRY ABB=ON PLU=ON L2
L4 STR



Structure attributes must be viewed using STN Express query preparation.

L6 118553 SEA FILE=REGISTRY SSS FUL L4
L7 QUE ABB=ON PLU=ON ?CYCLIZ? OR ?CYCLIS? OR (RING (2A) (C
LOS? OR FORM OR FORMING OR FORMS OR FORMATION))
L8 QUE ABB=ON PLU=ON ?CYCLODESUL? OR (CYCLO(W)DESUL?)
L9 QUE ABB=ON PLU=ON CYCLO (W) DE(W) (SULF? OR SULPH?)
L10 11576 SEA FILE=HCAPLUS ABB=ON PLU=ON L6
L11 2989 SEA FILE=HCAPLUS ABB=ON PLU=ON L6 (L) RACT+NT/RL
L12 652 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 (L) (L7 OR L8 OR L9)
L13 591 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND L12
L21 5 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND L3
L24 29 SEA FILE=HCAPLUS ABB=ON PLU=ON L21
L25 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L24 AND L13

Uploading loe105fulrxn.str



chain nodes :

1 2 3 4 7 8 9 27

ring nodes :

16 17 18 19 20 21 22

ring/chain nodes :

5 6

chain bonds :

1-2 2-3 2-9 3-4 4-5 6-7 7-8 18-27

ring/chain bonds :

5-6

ring bonds :

16-17 16-22 17-18 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 2-3 2-9 3-4 4-5 5-6 6-7 7-8 16-17 16-22 17-18 18-19 18-27 19-20

20-21 21-22

G1:O,S,N

G2:O,S,N

Connectivity :

9:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 16:Atom

17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 27:Atom

fragments assigned product role:

containing 16

fragments assigned reactant/reagent role:
containing 1

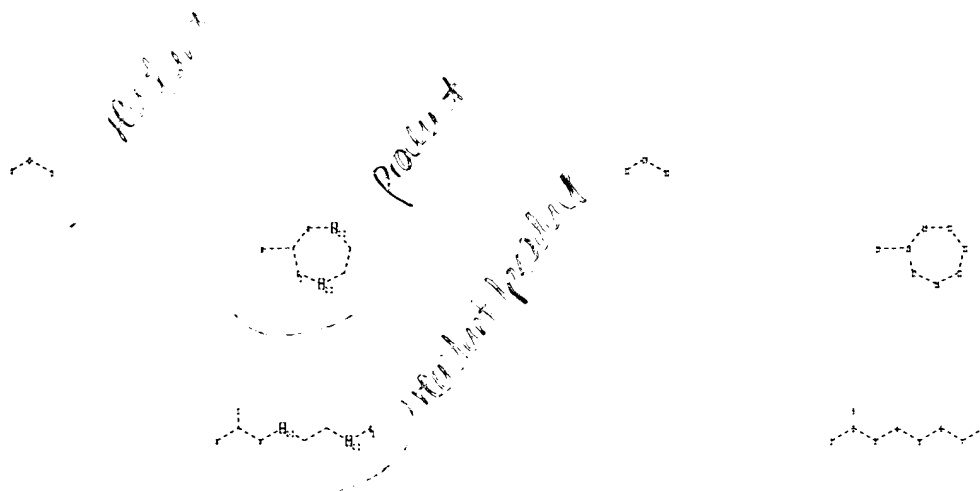
=> d que stat l33
L31 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L33 366 SEA FILE=CASREACT SSS FUL L31 (2195 REACTIONS)

100.0% DONE 22539 VERIFIED 2195 HIT RXNS 366 DOCS
SEARCH TIME: 00.00.08

Uploading loe105fulrxnr.str



chain nodes :

1 2 3 4 7 8 9 27 29 30 31

ring nodes :

16 17 18 19 20 21 22

ring/chain nodes :

5 6

chain bonds :

1-2 2-3 2-9 3-4 4-5 6-7 7-8 18-27 29-30 29-31

ring/chain bonds :

5-6

ring bonds :

16-17 16-22 17-18 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 2-3 2-9 3-4 4-5 5-6 6-7 7-8 16-17 16-22 17-18 18-19 18-27 19-20
20-21 21-22 29-30 29-31

G1:O,S,N

G2:O,S,N

Connectivity :

9:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 16:Atom
17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 27:Atom 29:Atom 30:Atom
31:Atom

fragments assigned product role:

containing 16

fragments assigned reactant/reagent role:

containing 1

containing 29

=> => d que stat l36

L31 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L33 366 SEA FILE=CASREACT SSS FUL L31 (2195 REACTIONS)

L34 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

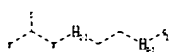
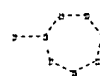
L36 61 SEA FILE=CASREACT SUB=L33 SSS FUL L34 (273 REACTIONS)

100.0% DONE 287 VERIFIED 273 HIT RXNS

61 DOCS

SEARCH TIME: 00.00.01

Uploading loe105fulrxnr.str



chain nodes :

1 2 3 4 7 8 9 27 29 30 31

ring nodes :

16 17 18 19 20 21 22

ring/chain nodes :

5 6

chain bonds :

1-2 2-3 2-9 3-4 4-5 6-7 7-8 18-27 29-30 29-31

ring/chain bonds :

5-6

ring bonds :

16-17 16-22 17-18 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 2-3 2-9 3-4 4-5 5-6 6-7 7-8 16-17 16-22 17-18 18-19 18-27 19-20
20-21 21-22 29-30 29-31

G1:O,S,N

G2:O,S,N

Connectivity :

9:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 16:Atom
17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 27:Atom 29:Atom 30:Atom
31:Atom

fragments assigned product role:

containing 16

fragments assigned reactant/reagent role:

containing 1

containing 29

=> d que stat 139
L34 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L39 18 SEA FILE=CHEMINFORMRX SSS FUL L34 (58 REACTIONS)

100.0% DONE 378 VERIFIED 58 HIT RXNS 18 DOCS
SEARCH TIME: 00.00.17

=> dup rem 125 136 139
DUPLICATE IS NOT AVAILABLE IN 'CHEMINFORMRX'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'HCAPLUS' ENTERED AT 11:01:02 ON 17 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CASREACT' ENTERED AT 11:01:02 ON 17 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CHEMINFORMRX' ENTERED AT 11:01:02 ON 17 JAN 2007
COPYRIGHT (C) FIZ-CHEMIE BERLIN
PROCESSING COMPLETED FOR L25
PROCESSING COMPLETED FOR L36
PROCESSING COMPLETED FOR L39
L47 82 DUP REM L25 L36 L39 (0 DUPLICATES REMOVED)
ANSWERS '1-3' FROM FILE HCAPLUS
ANSWERS '4-64' FROM FILE CASREACT
ANSWERS '65-82' FROM FILE CHEMINFORMRX

=> file stnguide
FILE 'STNGUIDE' ENTERED AT 11:02:46 ON 17 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 12, 2007 (20070112/UP).

=> d ibib ed ab hitstr

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' - CONTINUE?

(Y)/N:y

L47 ANSWER 1 OF 82 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1036708 HCAPLUS

DOCUMENT NUMBER: 142:23282

TITLE: Process for synthesizing heterocyclic compounds by reaction of diamines, amino alcohols, or amino thioalcohols with isothiocyanates and cyclization of thiourea intermediates

INVENTOR(S): Heinelt, Uwe; Lang, Hans-Jochen

PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany

SOURCE: U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004242560	A1	20041202	US 2004-840105	20040506
DE 10323701	A1	20041223	DE 2003-10323701	20030522
AU 2004240716	A1	20041202	AU 2004-240716	20040510
CA 2526646	A1	20041202	CA 2004-2526646	20040510
WO 2004103976	A2	20041202	WO 2004-EP4955	20040510
WO 2004103976	A3	20050210		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1631552	A2	20060308	EP 2004-731903	20040510
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004010565	A	20060620	BR 2004-10565	20040510
CN 1795178	A	20060628	CN 2004-80014178	20040510
NO 2005005991	A	20060214	NO 2005-5991	20051216
PRIORITY APPLN. INFO.:			DE 2003-10323701	A 20030522
			US 2003-507143P	P 20030930
			WO 2004-EP4955	W 20040510

OTHER SOURCE(S): MARPAT 142:23282

ED Entered STN: 03 Dec 2004

AB The invention provides the process for synthesizing heterocyclic compds. of formula (I) [X = S, O, NR5 (wherein R5 = H, C1-4 alkyl); m, o = 0, 1, 2; A = each (un)substituted Ph, naphthyl, or heteroaryl; R10-R17 = H, F, partially or fully fluorinated C1-4 alkyl; or R14 and R16 together are a bond, and R15 and R17, together with the two carbon atoms to which they

are bonded, form an aromatic six-membered carbocycle, in which one or two carbon atoms may be replaced by nitrogen, or a thiophene ring, wherein the aromatic six-membered carbocycle and the thiophene ring is optionally substituted; wherein, either (i) A is an aromatic ring system, or (ii) the ring formed from R15 and R17 is an aromatic system and m is zero, or (iii) each of A and the ring formed from R15 and R17 is an aromatic ring system] and their tautomers and their salts. In the process, an isothiocyanate of A-NCS (A = same as above) is initially reacted with a primary amine of formula (II) (R = H; m, o, X, R10-R17= same as above) to give a thiourea of formula II [R = A-NH-C(S)]. Subsequently, the thiourea II [R = A-NH-C(S)] is converted to the corresponding heterocycle I using a base and a sulfonyl chloride. Thus, a solution of Ph isothiocyanate (500 mg) in absolute THF (6 mL) was added dropwise over 20 min under argon to a solution of ethylenediamine (5.56 g) in absolute THF (6 mL) and the reaction mixture was treated with H₂O, acidified with 10% HCl, and extracted with EtOAc to give 50 mg 1-(2-aminoethyl)-3-phenylthiourea (III). III (50 mg) was dissolved in THF (1.5 mL) under argon, admixed with a solution of NaOH (25.6 mg) in H₂O (0.6 mL), and treated dropwise with a solution of p-toluenesulfonyl chloride (53.7 mg) in THF within 5 min. and the reaction mixture was stirred for 0.5 h to give, after workup and chromatog. purification, 20 mg 2-(phenylimino)imidazolidine.

IT 632356-19-5P 800378-35-2P

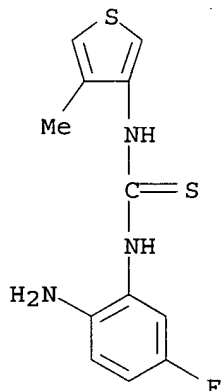
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(process for preparation of heterocyclic compds. by thiocarbamoylation of diamines or amino alcs. and cyclization of thiourea intermediates)

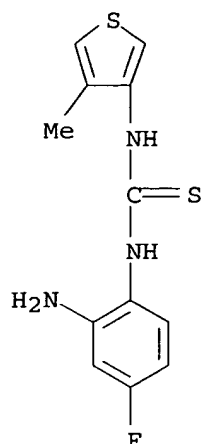
RN 632356-19-5 HCAPLUS

CN Thiourea, N-(2-amino-5-fluorophenyl)-N'-(4-methyl-3-thienyl)- (9CI) (CA INDEX NAME)



RN 800378-35-2 HCAPLUS

CN Thiourea, N-(2-amino-4-fluorophenyl)-N'-(4-methyl-3-thienyl)- (9CI) (CA INDEX NAME)



IT 29146-63-2P 31090-77-4P 800378-34-1P

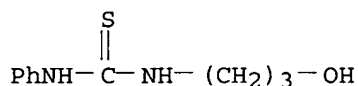
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(process for preparation of heterocyclic compds. by thiocarbamoylation of diamines, amino alcs., or amino thioalcs. and cyclization of thiourea intermediates)

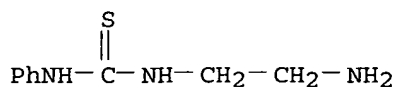
RN 29146-63-2 HCAPLUS

CN Thiourea, N-(3-hydroxypropyl)-N'-phenyl- (9CI) (CA INDEX NAME)



RN 31090-77-4 HCAPLUS

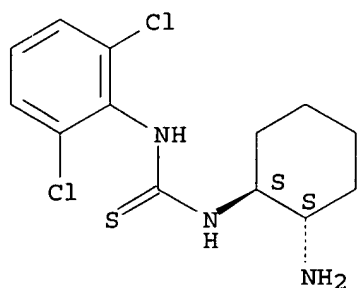
CN Thiourea, N-(2-aminoethyl)-N'-phenyl- (9CI) (CA INDEX NAME)



RN 800378-34-1 HCAPLUS

CN Thiourea, N-[(1R,2R)-2-aminocyclohexyl]-N'-(2,6-dichlorophenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



=> d ibib ed ab hitstr 2-3 .

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' - CONTINUE?
(Y)/N:y

L47 ANSWER 2 OF 82 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:122166 HCAPLUS

DOCUMENT NUMBER: 114:122166

TITLE: Synthesis and pharmacological investigations of
3-(aminoalkylene)-1-aryl-2-thioxo-4,5-
imidazolidinedione and 2,4,5-imidazolidinetrione
derivatives

AUTHOR(S): Zankowska-Jasinska, Wanda; Borowiec, Halina; Golus,
Janusz; Kolasa, Anna; Zaleska, Barbara; Krzywosinski,
Leszek; Bogdal, Maria; Przemyk, Barbara

CORPORATE SOURCE: Dep. Org. Chem., Jagiellonian Univ., Krakow, 30-060,
Pol.

SOURCE: Polish Journal of Pharmacology and Pharmacy (1990),
42(1), 49-58

CODEN: PJPPAA; ISSN: 0301-0244

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 06 Apr 1991

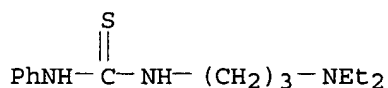
AB New derivs. of 2-thioxo-4,5-imidazolidinedione I (X = S; R = Ph;
3-MeOC₆H₄, 4-EtO₂CC₆H₄; NR₁R₂ = NH₂, N₂, 2,3-dioxopiperazinyl; n = 2, 3)
and 2,4,5-imidazolidinetrione I (X = O, R = Ph, R₁R₂ = N₂,
2,3-dioxopiperazinyl, n = 2) were synthesized by N,N'-acylation of asym.
thioureas and ureas by oxalyl chloride. I were screened for their central
action, mainly anticonvulsant activity, but showed no useful activity.

IT 730-19-8 889-28-1 31090-77-4

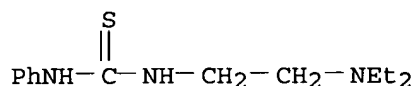
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with oxalyl chloride)

RN 730-19-8 HCAPLUS

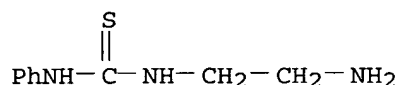
CN Thiourea, N-[3-(diethylamino)propyl]-N'-phenyl- (9CI) (CA INDEX NAME)



RN 889-28-1 HCAPLUS
 CN Thiourea, N-[2-(diethylamino)ethyl]-N'-phenyl- (9CI) (CA INDEX NAME)

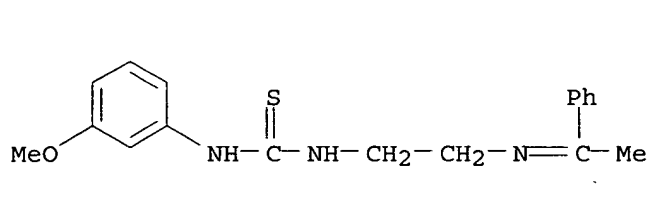


RN 31090-77-4 HCAPLUS
 CN Thiourea, N-(2-aminoethyl)-N'-phenyl- (9CI) (CA INDEX NAME)



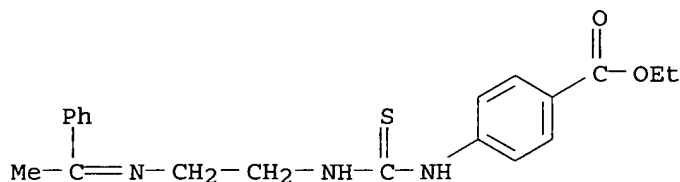
IT 132411-90-6P 132411-91-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)

RN 132411-90-6 HCAPLUS
 CN Thiourea, N-(3-methoxyphenyl)-N'-[2-[(1-phenylethylidene)amino]ethyl]-
 (9CI) (CA INDEX NAME)



*What numbered
 ring does this form?*

RN 132411-91-7 HCAPLUS
 CN Benzoic acid, 4-[[[2-[(1-phenylethylidene)amino]ethyl]amino]thioxomethyl]
 amino]-, ethyl ester (9CI) (CA INDEX NAME)



L47 ANSWER 3 OF 82 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1989:423460 HCAPLUS

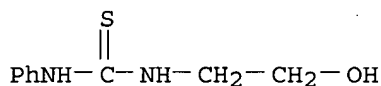
DOCUMENT NUMBER: 111:23460

TITLE: Reaction of phosphorous acid dialkylamides with
 N-(hydroxyalkyl)-N'-substituted thioureas. New
 synthesis of 2-iminothiazolidine and
 2-iminoperhydro-1,3-thiazine derivatives

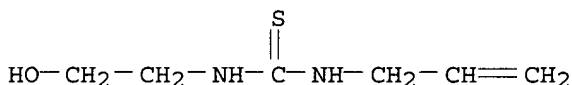
AUTHOR(S): Mizrakh, L. I.; Polonskaya, L. Yu.; Gvozdet'skii, A.
 N.; Vasil'ev, A. M.; Karpunina, L. B.

CORPORATE SOURCE: Inst. Biofiz., Moscow, USSR

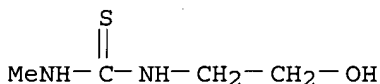
SOURCE: Zhurnal Obshchei Khimii (1988), 58(10), 2246-51
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 111:23460
 ED Entered STN: 21 Jul 1989
 AB Treatment of (hydroxyalkyl)thioureas RNHC(S)NR1(CH2)nCHR2OH (R = Me, Ph, alkyl; R1 = H, Me, CH2CH2OH; R2 = H, Me; n = 1, 2) with phosphorous acid dialkylamides P(NEt2)3 or (R3O)2PNet2 (R3 = Pr or R32 = CH2CH2) afforded title thiazolidine or thiazine derivs. I.
 IT 102-12-5 105-81-7 3120-26-1 5137-50-8
23309-78-6 29146-63-2 90914-63-9
109315-14-2 121215-87-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of in presence of phosphorous acid
 dialkylamide)
 RN 102-12-5 HCAPLUS
 CN Thiourea, N-(2-hydroxyethyl)-N'-phenyl- (9CI) (CA INDEX NAME)



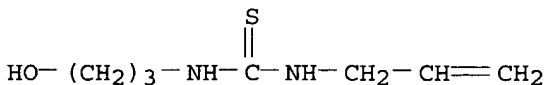
RN 105-81-7 HCAPLUS
 CN Thiourea, N-(2-hydroxyethyl)-N'-2-propenyl- (9CI) (CA INDEX NAME)



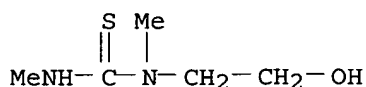
RN 3120-26-1 HCAPLUS
 CN Thiourea, N-(2-hydroxyethyl)-N'-methyl- (9CI) (CA INDEX NAME)



RN 5137-50-8 HCAPLUS
 CN Thiourea, N-(3-hydroxypropyl)-N'-2-propenyl- (9CI) (CA INDEX NAME)

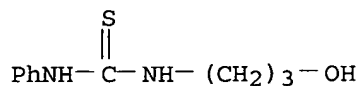


RN 23309-78-6 HCAPLUS
 CN Thiourea, N-(2-hydroxyethyl)-N,N'-dimethyl- (9CI) (CA INDEX NAME)



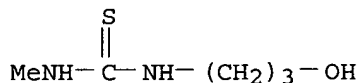
RN 29146-63-2 HCAPLUS

CN Thiourea, N-(3-hydroxypropyl)-N'-phenyl- (9CI) (CA INDEX NAME)



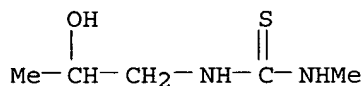
RN 90914-63-9 HCAPLUS

CN Thiourea, N-(3-hydroxypropyl)-N'-methyl- (9CI) (CA INDEX NAME)



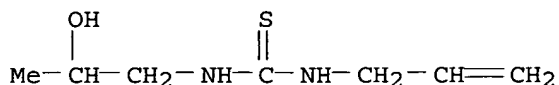
RN 109315-14-2 HCAPLUS

CN Thiourea, N-(2-hydroxypropyl)-N'-methyl- (9CI) (CA INDEX NAME)



RN 121215-87-0 HCAPLUS

CN Thiourea, N-(2-hydroxypropyl)-N'-(2-propenyl)- (9CI) (CA INDEX NAME)

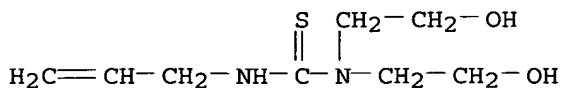


IT 5137-48-4P 121215-67-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)

RN 5137-48-4 HCAPLUS

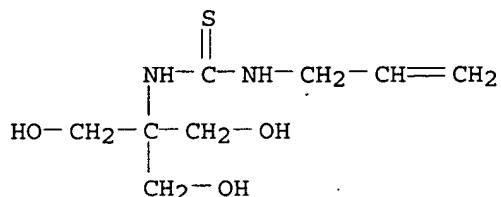
CN Thiourea, N,N-bis(2-hydroxyethyl)-N'-2-propenyl- (9CI) (CA INDEX NAME)



RN 121215-67-6 HCAPLUS

CN Thiourea, N-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-N'-2-propenyl- (9CI)

(CA INDEX NAME)



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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' - CONTINUE?
(Y)/N:y

'ED' IS NOT A VALID FORMAT

REENTER DISPLAY FORMAT FOR ALL FILES (FILEDEFAULT):ibib ab fhit

L47 ANSWER 4 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:210938 CASREACT

TITLE: Aminothiazole derivatives as neuropeptide Y5 receptor
ligands: finding the balance between affinity and
physicochemical properties

AUTHOR(S): Nettekoven, Matthias; Guba, Wolfgang; Neidhart,
Werner; Mattei, Patrizio; Pflieger, Philippe;
Plancher, Jean-Marc; Taylor, Sven

CORPORATE SOURCE: Pharmaceutical Research Basel, Discovery Chemistry, F.
Hoffmann-La Roche Ltd., Basel, 4070, Switz.

SOURCE: ChemMedChem (2006), 1(1), 45-48

CODEN: CHEMGX; ISSN: 1860-7179

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

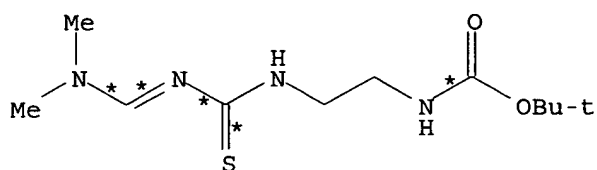
DOCUMENT TYPE: Journal

LANGUAGE: English

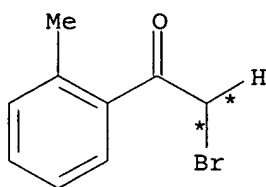
AB A straight-forward parallel solution-phase synthesis of novel thiazole
derivs. I (X = 1,2-ethylene, 1,3-propylene, 1,4-phenylene, etc.; R1 =
Me2N, 2-FC6H4, 4-MeOC6H4, 2-thienyl; R2 = H, Me) with varying linker
moieties is described. Assessments of artificial membrane permeability
and solubility show that some members of this compound class may be suitable
antagonists for the neuropeptide Y5 receptor, which is involved in the
stimulation of food intake.

RX(69) OF 144 COMPOSED OF RX(49), RX(1)

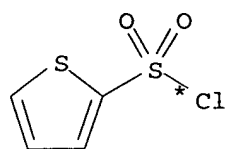
RX(69) BH + CA + B ==> C



BH

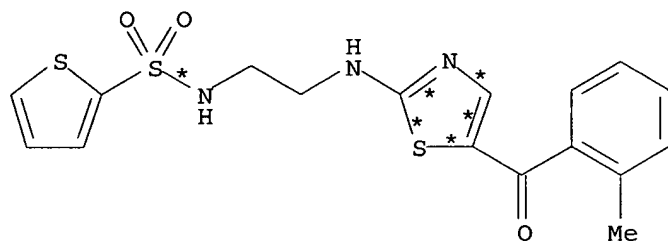


CA



B

2
STEPS
→



C

RX(49) RCT BH 593270-45-2, CA 51012-65-8
 RGT E 121-44-8 Et3N
 PRO A 593270-46-3
 SOL 64-17-5 EtOH
 CON 16 hours, 100 deg C

RX(1) RCT A 593270-46-3

STAGE(1)

RGT D 7647-01-0 HCl
 SOL 123-91-1 Dioxane
 CON room temperature

STAGE(2)

RCT B 16629-19-9
 RGT E 121-44-8 Et3N
 SOL 67-56-1 MeOH, 75-09-2 CH2Cl2
 CON 16 hours, 50 deg C

PRO C 593269-65-9

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib ab fhit 5-64

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' - CONTINUE?
(Y)/N:y

L47 ANSWER 5 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:336517 CASREACT
TITLE: Preparation of 17-heterocyclic-4-aza-5 α -androst-1-en-3-one derivatives for their use as modulators of the androgen receptor in a tissue selective manner
INVENTOR(S): Kaufman, Mildred L.; Meissner, Robert S.; Mitchell, Helen J.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005025572	A1	20050324	WO 2004-US28655	20040902
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW</p> <p>RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				
AU 2004272007	A1	20050324	AU 2004-272007	20040902
CA 2537660	A1	20050324	CA 2004-2537660	20040902
EP 1663228	A1	20060607	EP 2004-783033	20040902
<p>R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK</p>				
CN 1849120	A	20061018	CN 2004-80025867	20040902
PRIORITY APPLN. INFO.:			US 2003-501789P	20030910
			WO 2004-US28655	20040902

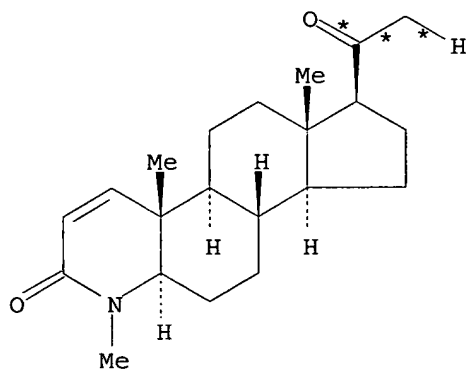
OTHER SOURCE(S): MARPAT 142:336517

AB 17-Heterocyclic-4-aza-5 α -androst-1-en-3-one derivs., such as I [dashed bond = single bond, double bond; X = H, halo; Y, Z = H, alkyl, halo; Y and Z, together with the carbon atom to which they are attached = cyclopropyl; n = 0-3; U, V, W, D = CH, N, S, O; R1 = H, CF3, carbonyl(alkyl), OH, alkoxy, halo, alkyl, CH2OH, alkylamino; R2 = halo, carbonyl(alkyl), carbonyl(alkenyl), carbonyl(alkynyl), alkenylamino, heterocyclic, etc.], were prepared for their use as modulators of the androgen receptor (AR) in a tissue selective manner. Thus, II (R = OH) was treated with Et3N, and iso-Bu chloroformate, followed by reaction with

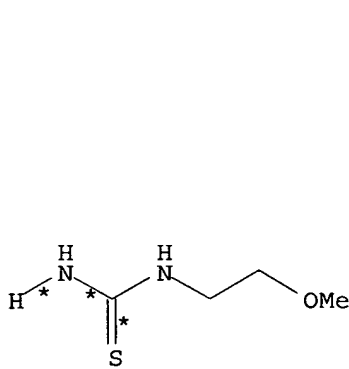
N,O-dimethylhydroxylamine hydrochloride to give II [R = N(Me)OMe (III)]. III was converted to 4-aza-5 α -androst-1-en-3,20-dione derivative II (R = Me), and then to bromide II [R = CH₂Br (IV)], which was treated with N-butyl-thiourea to afford V. The prepared compds. are useful in the enhancement of weakened muscle tone and the treatment of conditions caused by androgen deficiency or which can be ameliorated by androgen administration, including osteoporosis, osteopenia, glucocorticoid-induced osteoporosis, periodontal disease, bone fracture, bone damage following bone reconstructive surgery, sarcopenia, frailty, aging skin, male hypogonadism, postmenopausal symptoms in women, atherosclerosis, hypercholesterolemia, hyperlipidemia, obesity, aplastic anemia and other hematopoietic disorders, inflammatory arthritis and joint repair, HIV-wasting, prostate cancer, benign prostatic hyperplasia (BPH), abdominal adiposity, metabolic syndrome, type II diabetes, cancer cachexia, Alzheimer's disease, muscular dystrophies, cognitive decline, sexual dysfunction, sleep apnea, depression, premature ovarian failure, and autoimmune disease, alone or in combination with other active agents.

RX(125) OF 329 COMPOSED OF RX(78), RX(11)

RX(125) FJ + W ==> X

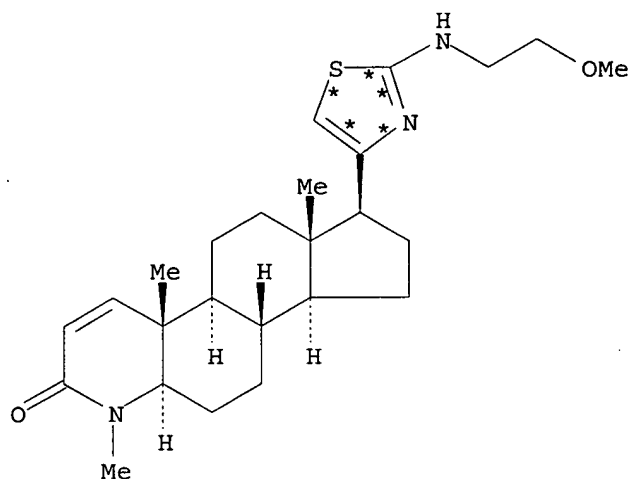


FJ



W

2
STEPS
→



X

RX(78) RCT FJ 848354-06-3

STAGE(1)

RGT FM 7726-95-6 Br2

SOL 67-56-1 MeOH

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature

SUBSTAGE(3) 18 hours, room temperature

STAGE(2)

RGT FN 7631-90-5 NaHSO3

SOL 7732-18-5 Water

CON room temperature

PRO A 848354-07-4

RX(11) RCT W 102353-42-4, A 848354-07-4PRO X 848353-39-9

SOL 64-17-5 EtOH

CON 14 hours, room temperature

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 6 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:477631 CASREACT

TITLE: Solid-Phase and Solution-Phase Syntheses of Oligomeric
Guanidines Bearing Peptide Side Chains

AUTHOR(S): Zhang, Zhongsheng; Fan, Erkang

CORPORATE SOURCE: Department of Biochemistry, Biomolecular Structure
Center, University of Washington, Seattle, WA, 98195,
USA

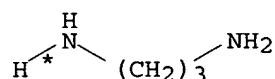
SOURCE: Journal of Organic Chemistry (2005), 70(22), 8801-8810
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

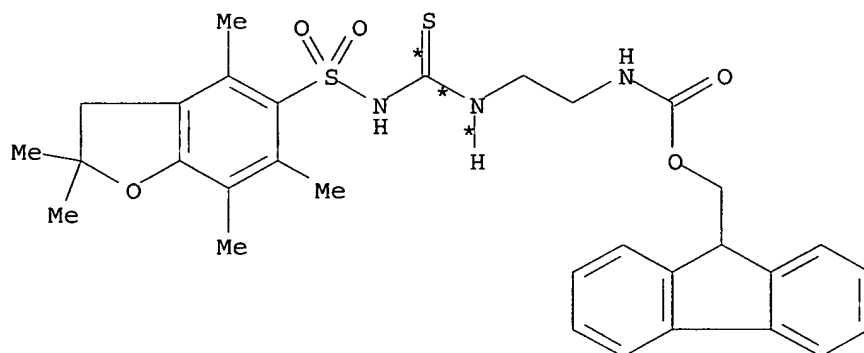
DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Synthetic strategies for preparing N,N'-bridged oligomeric guanidines bearing peptide side chains both on solid support and in solution are presented. Monomers are prepared from common amino acids and therefore contain conventionally protected peptide side chains. The side chains include alkyl, aromatic, hydroxyl, amino, carboxylic acid and amide functional groups. Oligomer elongation utilizes acid-sensitive sulfonyl activated thiourea through the formation of carbodiimide intermediate. With proper preparation of monomers, synthesis of oligomer can be performed in two directions (equivalent to N to C terminal or C to N terminal in a peptide sequence) with excellent efficiency. 192 Mg of guanidine-based oligomer I, as a trifluoroacetate salt, was synthesized via solid-phase synthesis methods performed in N to C terminal direction.

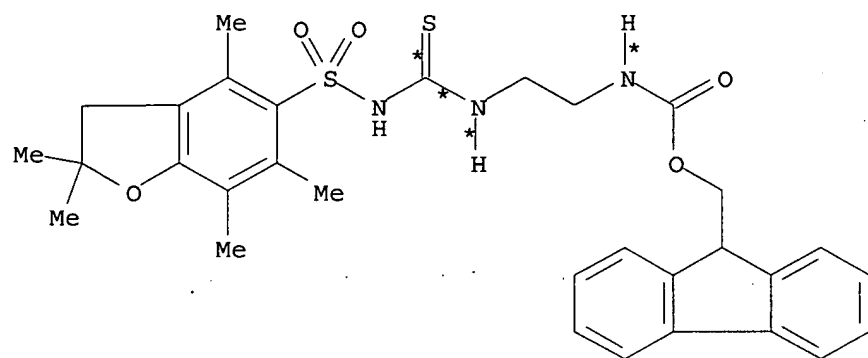
RX(15) OF 159 ...AM + 2 AL ==> AN + AO...



AM
 resin-bound

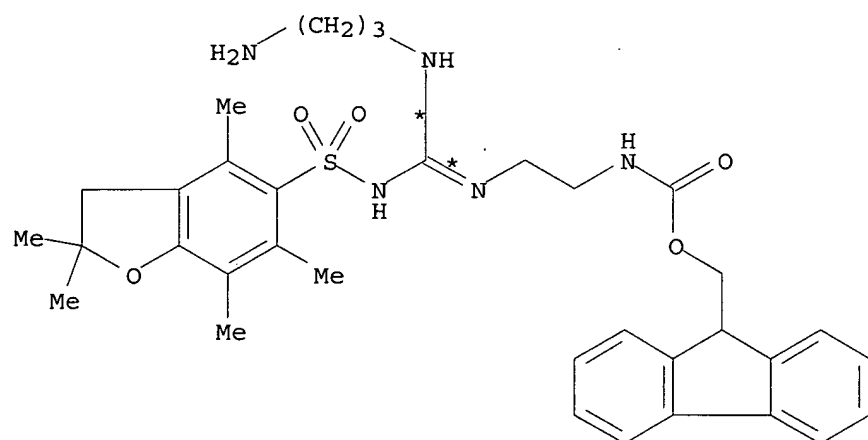


AL

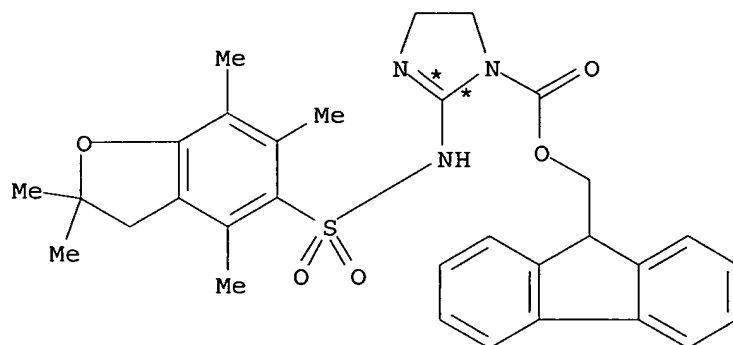


AL

(15) →



AN
YIELD 29%
resin-bound



AO
YIELD 94%

RX(15) RCT AM 109-76-2D

STAGE(1)

SOL 75-09-2 CH₂Cl₂
CON 2 hours, room temperature

STAGE(2)

RGT AP 67-56-1 MeOH
CON room temperature

STAGE(3)

RCT AL **869735-78-4**
RGT Z 7087-68-5 EtN(Pr-i)₂, AA 25952-53-8 EDAP
SOL 75-09-2 CH₂Cl₂
CON overnight, room temperature

STAGE(4)

RGT AQ 82911-69-1 2,5-Pyrrolidinedione, 1-[[[(9H-fluoren-9-ylmethoxy)carbonyl]oxy]-, Z 7087-68-5 EtN(Pr-i)₂
SOL 75-09-2 CH₂Cl₂
CON overnight, room temperature

STAGE(5)

RGT AE 6485-79-6 Silane, tris(1-methylethyl)-, AF 7732-18-5
Water, W 76-05-1 F₃CCO₂H
SOL 7732-18-5 Water, 76-05-1 F₃CCO₂H
CON 2 hours, room temperature

PRO AN 869735-87-5D, AO **869735-88-6**

NTE solid-supported reaction, first stage is attachment to trityl chloride resin

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 7 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:88225 CASREACT

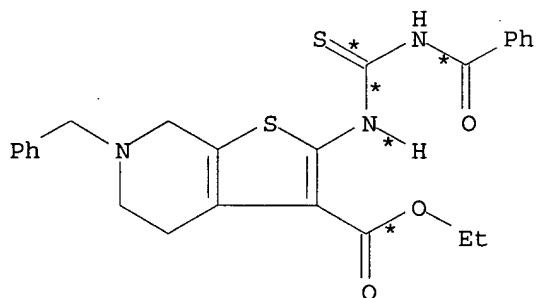
TITLE: Synthesis of Tricyclic 1,3-Oxazin-4-ones and Kinetic

Analysis of Cholesterol Esterase and
Acetylcholinesterase Inhibition

AUTHOR(S): Pietsch, Markus; Guetschow, Michael
CORPORATE SOURCE: Pharmaceutical Institute, University of Bonn, Bonn,
D-53115, Germany
SOURCE: Journal of Medicinal Chemistry (2005), 48(26),
8270-8288
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

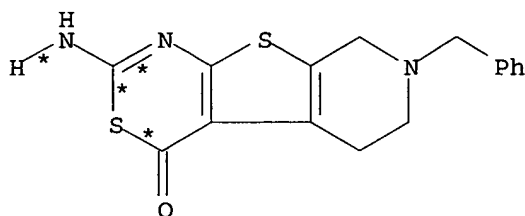
AB A series of thieno[1,3]oxazin-4-ones and thieno[1,3]thiazin-4-ones were synthesized and investigated as inhibitors of the α/β hydrolases cholesterol esterase (CEase) and acetylcholinesterase (AChE). The introduction of a cycloaliph. five- or six-membered ring fused at the thiophene was favorable for CEase inhibition. Such compds. were analyzed as true alternate substrate inhibitors. 6,7-Dihydro-2-(dimethylamino)-4H,5H-cyclopenta[4,5]thieno[2,3-d][1,3]oxazin-4-one (I) exhibited a K_i value of 630 nM and excelled in its low susceptibility to CEase-catalyzed degradation. I and its analogs did not inhibit AChE. The introduction of a tetrahydropyrido ring with bulky hydrophobic substituents at the basic nitrogen provided inhibitors of AChE which were completely inactive toward CEase. 7-Benzyl-5,6,7,8-tetrahydro-2-(N-3,4-dimethoxybenzyl-N-methylamino)-4H-pyrido[4',3':4,5]thieno[2,3-d][1,3]oxazin-4-one had the IC_{50} value of 330 nM for AChE inhibition. A residual enzymic activity at an infinite inhibitor concentration and thus a catalytically active ternary enzyme-substrate-inhibitor complex was concluded. To specify kinetic parameters of inhibition, a new method was derived to characterize selected thieno[1,3]oxazin-4-ones as hyperbolic mixed-type inhibitors of AChE.

RX(42) OF 103 CJ ==> CK



CJ

(42)



CK

RX(42) RCT CJ 102609-55-2

STAGE(1)

RGT CL 7664-93-9 H2SO4
 SOL 7732-18-5 Water
 CON room temperature - 100 deg C

STAGE(2)

RGT CM 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON 0 deg C

PRO CK 117516-95-7

REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 8 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:229771 CASREACT

TITLE: Isomeric thiazole derivatives as ligands for the
neuropeptide Y5 receptorAUTHOR(S): Nettekoven, Matthias; Guba, Wolfgang; Neidhart,
Werner; Mattei, Patrizio; Pflieger, Philippe; Roche,
Olivier; Taylor, SvenCORPORATE SOURCE: Pharmaceutical Research Basel, Discovery Chemistry, F.
Hoffmann-La Roche Ltd., Basel, CH-4070, Switz.SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),
15(14), 3446-3449
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

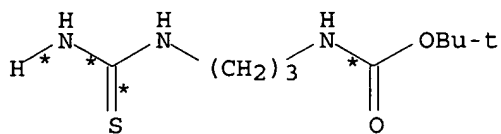
DOCUMENT TYPE: Journal

LANGUAGE: English

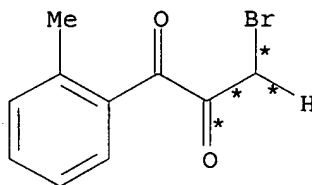
AB Sets of isomeric thiazoles I [R = 4-FC6H4, 3-MeOC6H4, 2,5-(MeO)2C6H3,
2-furyl, etc.] and II have been synthesized in a parallel iterative
solution-phase synthesis approach guided by the SAR anal. derived from biol.
results and computer-aided design and anal. This synergistic and
streamlined working procedure led to highly active isomeric NPY5 receptor
ligands. However, a 10-fold difference at least in their resp. binding
affinities was consistently found for all isomeric pairs I and II. The
anal. of conformational differences due to heteroatom interactions in I
and II revealed a favorable C=O...S interaction in I,
whereas thiazoles II showed a repulsive C=O...N
interaction.

RX(19) OF 39 COMPOSED OF RX(2), RX(10)

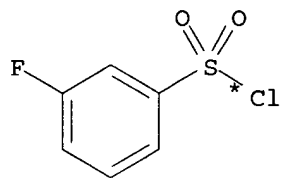
RX(19) A + D + I ==> Y



A

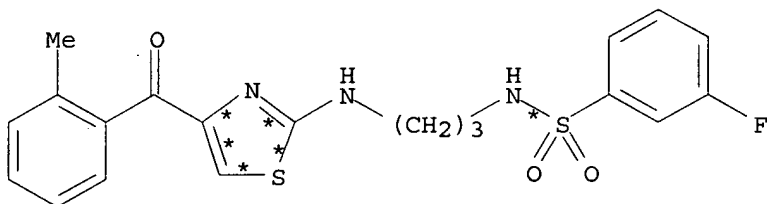


D



I

2
STEPS
→



Y

RX(2) RCT A 270260-72-5, D 82102-48-5
RGT F 121-44-8 Et3N
PRO E 593269-10-4
SOL 67-56-1 MeOH
CON 2 hours, 80 deg C

RX(10) RCT E 593269-10-4

STAGE(1)

RGT K 7647-01-0 HCl
SOL 123-91-1 Dioxane

STAGE(2)

RCT I 701-27-9

PRO Y 593269-24-0

REFERENCE COUNT: 10

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Loewe *no new info*

L47 ANSWER 9 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:229950 CASREACT

TITLE: Diazaallyls of group 4 metals based on trans-1,2-diaminocyclohexane

AUTHOR(S): Crust, Edward J.; Munslow, Ian J.; Scott, Peter

CORPORATE SOURCE: Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK

SOURCE: Journal of Organometallic Chemistry (2005), 690(14), 3373-3382

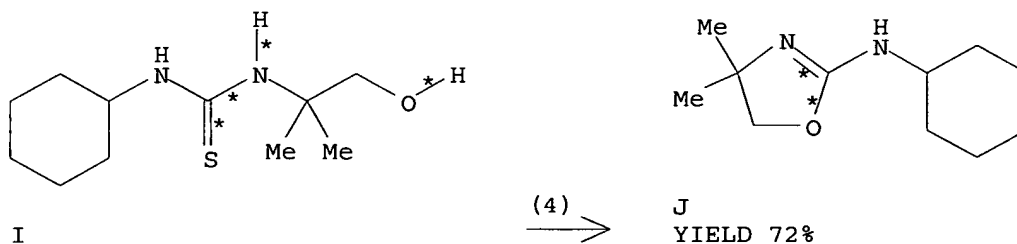
CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Amination of 2-bromo-6-methylpyridine with trans-1,2-diaminocyclohexane gives the corresponding bis(aminopyridine) H2L1. Conversion of the same diamine to the N,N'-bis(amino-4,4-dimethylthiazoline) H2L2 is also completed in three steps. The analogous aminooxazoline is, however, inaccessible, although the aminocyclohexane analog was prepared readily. The proligand H2L1 forms bis(aminopyridinato) alkyl complexes [ZrL1R2] (R = CH2Ph, CH2But). The mol. structure of the neopentyl complex shows that the chiral backbone leads to a puckering of the N4Zr coordination sphere, which contrasts with the related cyclohexyl-bridged Schiff-base complexes which are essentially planar. [ZrL2(CH2But)2] - the 1st aminothiazolinato complex - is formed similarly. A comparison of the structures of [ZrL1(CH2But)2] and [ZrL2(CH2But)2] indicates that the latter has a fully delocalized N-C-N system, rather similar to a bis(amidinate). Reaction of H2L2 with [Ti(NMe2)4] gives [TiL2(NMe2)2] which appears to be C2-sym. like the above complexes according to NMR spectra, but has one uncoordinated thiazoline unit in the solid state. This is a result of increased ring strain at the smaller Ti metal center.

RX(4) OF 22 ...I ==> J

RX(4) RCT I 66450-69-9
RGT K 1310-73-2 NaOH, L 104-15-4 TsOH
PRO J 862672-75-1
SOL 7732-18-5 Water, 109-99-9 THF
CON SUBSTAGE(1) 20 minutes, room temperature
SUBSTAGE(2) overnight, room temperature

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 10 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:331743 CASREACT

TITLE: Metal-Free Catalysts for the Hydrolysis of RNA Derived from Guanidines, 2-Aminopyridines, and 2-Aminobenzimidazoles

AUTHOR(S): Scheffer, Ute; Strick, Andreas; Ludwig, Verena; Peter, Sascha; Kalden, Elisabeth; Goebel, Michael W.

CORPORATE SOURCE: Institute for Organic Chemistry and Chemical Biology, Goethe-University Frankfurt, Frankfurt am Main, 60439, Germany

SOURCE: Journal of the American Chemical Society (2005), 127(7), 2211-2217

CODEN: JACSAT; ISSN: 0002-7863

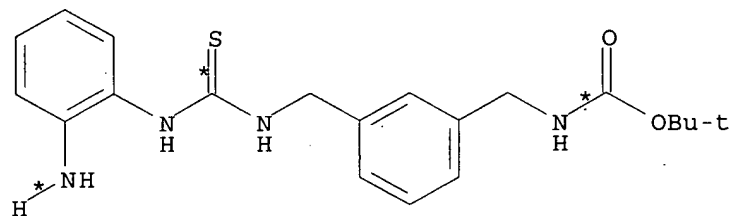
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

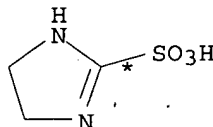
LANGUAGE: English

AB 2-Aminopyridine and 2-aminobenzimidazole were chosen as structural analogs to substitute guanidinium groups in receptor mols. designed as phosphoryl transfer catalysts. Shifting the pKa of the guanidinium analogs toward 7 was expected to raise catalytic activities in aqueous buffer. Although the pKa's of both heterocycles are similar (6.2 and 7.0), only 2-aminobenzimidazole led to active RNA cleavers. All cleavage assays were run with fluorescently labeled substrates and a DNA sequencer. RNase contaminations would degrade RNA enantioselectively. In contrast, achiral catalysts such as 9b and 10b necessarily induce identical cleavage patterns in RNA and its mirror image. This principle allowed the authors to safely rule out contamination effects in this study. The most active catalysts, tris(2-aminobenzimidazoles) 9b and 10b, were shown by fluorescence correlation spectroscopy (FCS) to aggregate with oligonucleotides. However, at very low concns. the compds. are still active in the nonaggregated state. Conjugates of 10b with antisense oligonucleotides or RNA binding peptides, therefore, will be promising candidates as site specific artificial RNases.

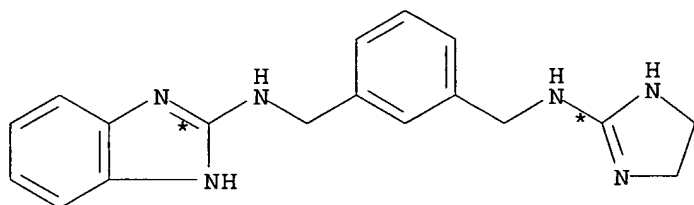
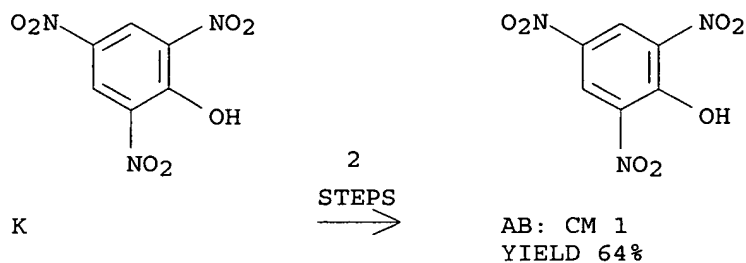
RX(24) OF 44 COMPOSED OF RX(6), RX(7)

RX(24) Z + J + K ==> AB

Z



J



AB: CM 2
YIELD 64%

RX (6) RCT Z 848408-57-1
 RGT V 21908-53-2 HgO
 PRO AA 848408-58-2
 CAT 7704-34-9 S
 SOL 64-17-5 EtOH
 CON 2 hours, room temperature -> reflux

RX (7) RCT AA 848408-58-2

STAGE (1)

RGT F 7647-01-0 HCl
 SOL 67-56-1 MeOH
 CON room temperature

STAGE (2)

RCT J 64205-92-1
 RGT M 121-44-8 Et3N
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON 8 hours, room temperature

STAGE (3)

RCT K 88-89-1
 SOL 67-56-1 MeOH
 CON reflux

PRO AB 848408-72-0

REFERENCE COUNT: 62

THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 11 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:188927 CASREACT

TITLE: Synthesis, inhibition properties, and theoretical study of the new nanomolar trehalase inhibitor 1-thiatrehazolin: Towards a structural understanding of trehazolin inhibition

AUTHOR(S): Chiara, Jose Luis; Storch de Gracia, Isabel; Garcia, Angela; Bastida, Agatha; Bobo, Sofia; Martin-Ortega, Maria D.

CORPORATE SOURCE: Instituto de Quimica Organica General, CSIC, Madrid, 28006, Spain

SOURCE: ChemBioChem (2005), 6(1), 186-191

CODEN: CBCHFX; ISSN: 1439-4227

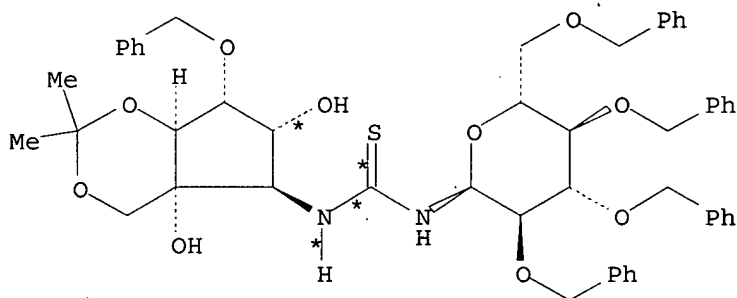
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

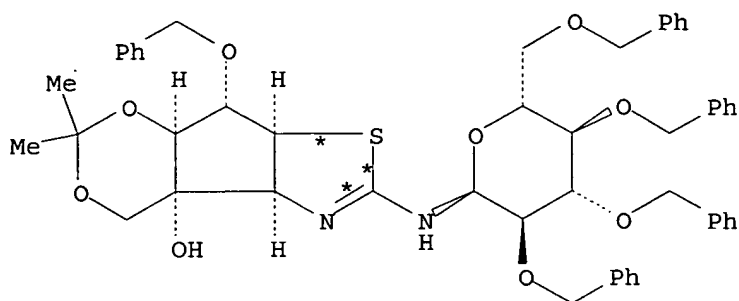
AB A new trehazolin analog, 1-thiatrehazolin, has been synthesized from carbohydrate precursors by a highly efficient route based on our previously developed ketone/oxime ether reductive carbocyclization reaction for the construction of the cyclitol ring and an intramol. nucleophilic displacement reaction for the construction of the thiazoline ring. 1-Thiatrehazolin is a very potent, slow, tight-binding trehalase inhibitor. A structural model for trehalase inhibition by trehazolin and its analogs, based on the exptl. results and supported by theor. calcns., is proposed.

RX(2) OF 10 ...C ==> E...



C

(2) →



E
YIELD 93%

RX(2) RCT C 252209-36-2
RGT F 110-86-1 Pyridine, G 358-23-6 (F3CSO2)2O
PRO E 861896-97-1
SOL 75-09-2 CH2Cl2
CON 1 hour, -40 deg C

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 12 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:410834 CASREACT

TITLE: A convenient method for the synthesis of 2-amino substituted aza-heterocycles from N,N'-disubstituted thioureas using TsCl/NaOH

AUTHOR(S): Heinelt, Uwe; Schultheis, Daniela; Jaeger, Siegfried; Lindenmaier, Marion; Pollex, Annett; Beckmann, Henning S. G.

CORPORATE SOURCE: Chemistry, Aventis, Frankfurt, 65926, Germany

SOURCE: Tetrahedron (2004), 60(44), 9883-9888

CODEN: TETRAB; ISSN: 0040-4020

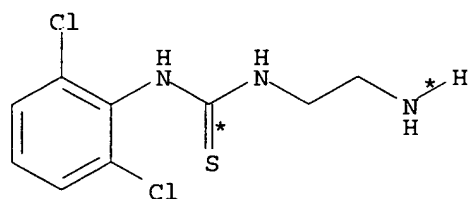
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

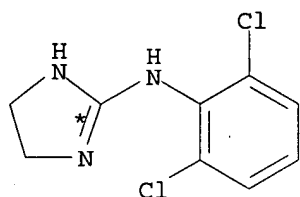
LANGUAGE: English

AB P-Toluenesulfonyl chloride (TsCl)/NaOH has been introduced as reagent combination for the synthesis of 2-aminooxazolidines or 2-aminothiazolidines from N-(2-hydroxyethyl)thioureas, but its general application in heterocycle synthesis has not been investigated. In this paper the convenient and efficient synthesis of a variety of 2-amino-substituted 1-aza-3-(aza, oxa or thia) heterocycles of different substitution and ring sizes is described. The application of polymer-supported TsCl facilitates work-up and renders the reaction conditions very suitable for parallel or robot synthesis.

RX(7) OF 28 ...M ==> X



M



X

YIELD 60%

RX(7) RCT M 65295-68-3

STAGE(1)

RGT F 98-59-9 TsCl, G 1310-73-2 NaOH

SOL 7732-18-5 Water, 109-99-9 THF

CON SUBSTAGE(1) 1 hour, room temperature

SUBSTAGE(2) overnight, room temperature

STAGE(2)

SOL 75-09-2 CH₂Cl₂PRO X 4205-90-7

NTE solid-supported reagent, ps -bound TsCl

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACINTED

L47 ANSWER 13 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:411028 CASREACT

TITLE: Chiral Complexes of a New Diazaallyl Ligand: Group 4
Aminooxazolinates

AUTHOR(S): Westmoreland, Ian; Munslow, Ian J.; Clarke, Adam J.;
Clarkson, Guy; Scott, Peter

CORPORATE SOURCE: Department of Chemistry, University of Warwick,
Coventry, CV4 7AL, UK

SOURCE: Organometallics (2004), 23(21), 5066-5074
CODEN: ORGN7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

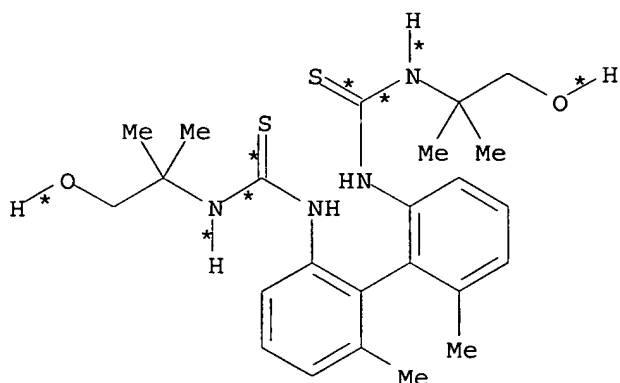
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new biaryl-bridged bis(iminooxazolidine) proligand (I; H₂L) was prepared

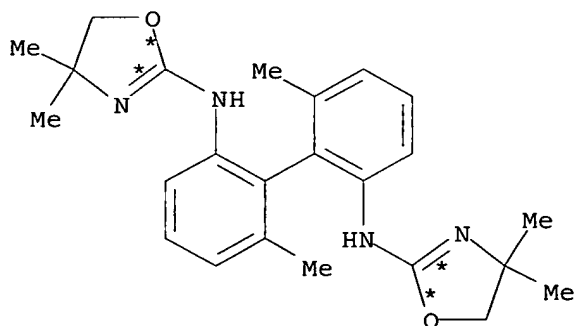
in good yield from 2,2-diamino-6,6'-dimethylbiphenyl. The direct reaction of H2L with $[\text{Ti}(\text{CH}_2\text{Ph})_4]$ leads via deprotonation of the ligand to the C2-sym. dibenzyl complex $[\text{LTi}(\text{CH}_2\text{Ph})_2]$ (85%) containing diazaallyl ligation. The analogous Group IVB $[\text{LZr}(\text{CH}_2\text{Ph})_2]$ (79%) and $[\text{LHf}(\text{CH}_2\text{Ph})_2]$ (91%) are similarly obtained. Mol. structures of these three compds. indicate C2-symmetry in all cases and that the chirality of the backbone is well expressed in the coordination sphere. Reaction of H2L with $\text{Ti}(\text{NMe}_2)_4$ gives the amide $[\text{LTi}(\text{NMe}_2)_2]$ (90%), which on reaction with SiMe_3Cl gives the chloride $[\text{LTiCl}_2]$ (78%). The dichloride $[\text{LZr}(\text{NMe}_2\text{H})\text{Cl}_2]$ was prepared via treatment of H2L with $\text{Zr}(\text{NMe}_2)_2\text{Cl}_2(\text{THF})_2$ (86%). The direct reaction of H2L with $\text{TiCl}_4(\text{THF})_2$ gives $[(\text{H}_2\text{L})\text{TiCl}_4]$ (83%), which is shown by x-ray crystallog. to contain intramol. $\text{NH}\cdots\text{Cl}$ H bond contacts. The complexes were tested as precatalysts for the polymerization of ethene and 1-hexene using a range of cocatalysts and display low activity. Correspondingly, NMR studies on a presumed active species $[\text{LZr}(\text{CH}_2\text{Ph})][\text{B}(\text{C}_6\text{F}_5)_3(\text{CH}_2\text{Ph})]$ were consistent with tight ion pairing on the NMR chemical shift time scale.

RX(3) OF 34 ...F ==> H...



F

(3) →



H
YIELD 85%

RX(3) RCT F 792934-58-8

STAGE(1)

SOL 109-99-9 THF
CON room temperature

STAGE(2)

RGT I 1310-73-2 NaOH, J 98-59-9 TsCl
SOL 7732-18-5 Water, 109-99-9 THF
CON 15 hours, room temperature

PRO H 792934-59-9

NTE in the dark

REFERENCE COUNT: 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L47 ANSWER 14 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:332151 CASREACT

TITLE: A 1,3-Diaza-Claisen Rearrangement that Affords
Guanidines

AUTHOR(S): Bowser, Amy M.; Madalengoitia, Jose S.

CORPORATE SOURCE: Department of Chemistry, University of Vermont,
Burlington, VT, 05405, USA

SOURCE: Organic Letters (2004), 6(19), 3409-3412

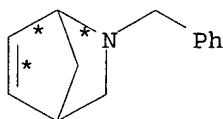
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

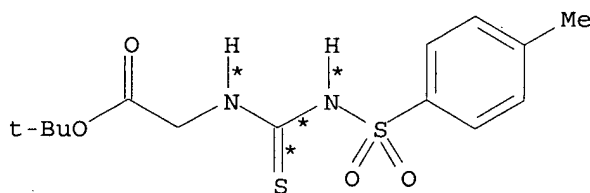
DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-Alkyl-N'-tosylthioureas activated by EDCI react with azanorbonenes at
room temperature through a 1,3-diaza-Claisen rearrangement, affording highly
substituted, bicyclic guanidines in moderate to good yields. Thus, the
diaza-Claisen rearrangement of 2-(phenylmethyl)-2-azabicyclo[2.2.1]hept-5-
ene (I) 4-methyl-N-[[[(phenylmethyl)amino]thioxomethyl]benzenesulfonamide
(N-benzyl-N'-tosylthiourea) (II) gave a bicyclic guanidine derivative (III).

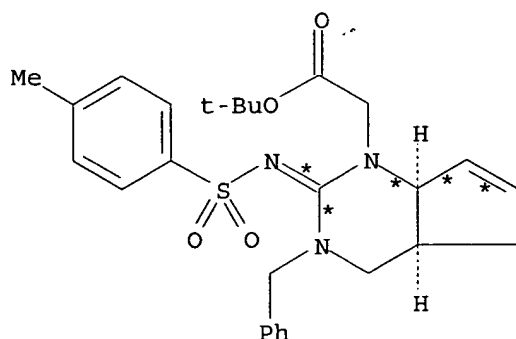
RX(13) OF 42 ...D + R ==> AA

D



R

(13) →



AA

YIELD 71%

RX(13) RCT D 112375-05-0, R 773147-12-9
 RGT S 7087-68-5 EtN(Pr-i)₂, X 25952-53-8 EDAP
 PRO AA 773147-16-3
 SOL 67-66-3 CHCl₃
 CON overnight, room temperature
 NTE regioselective, stereoselective, zwitterionic 1,3-diaza-Claisen rearrangement

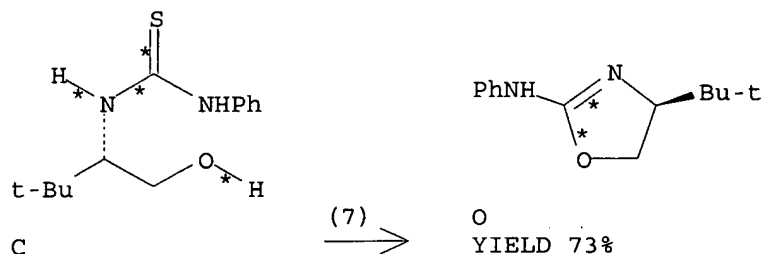
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~PRINTED~~
 L47 ANSWER 15 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:114243 CASREACT
 TITLE: Aminooxazolate; a chiral amidinate analogue
 AUTHOR(S): Munslow, Ian J.; Wade, Andrew R.; Deeth, Robert J.; Scott, Peter
 CORPORATE SOURCE: Department of Chemistry, University of Warwick, Coventry, UK
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2004), (22), 2596-2597
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB High levels of diastereoselection with respect to chirality-at-metal are achieved at equilibrium for complexes containing a new and available range of diazaallyl ligands. For example, (S)-2-(3,5-dimethyl)phenylamino-4-tert-butyloxazoline (HL) was prepared and reacted with Zr(CH₂Ph)₄ giving (Δ,SC)-[ZrL₂(CH₂Ph)₂] (1) in 84% yield. The structure of 1 was established by x-ray crystallog. and DFT calcns.

RX(7) OF 38 ...C ==> O...



RX(7) RCT C 821775-10-4
 RGT P 1310-73-2 NaOH, Q 98-59-9 TsCl
 PRO O 821775-06-8
 SOL 7732-18-5 Water, 109-99-9 THF
 CON SUBSTAGE(1) 5 minutes, room temperature
 SUBSTAGE(2) overnight, room temperature
 REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 16 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:143331 CASREACT

TITLE: Design and synthesis of 1,5- and 2,5-substituted
 tetrahydrobenzazepinones as novel potent and selective
 integrin $\alpha V\beta 3$ antagonists

AUTHOR(S): Kling, Andreas; Backfisch, Gisela; Delzer, Jurgen;
 Geneste, Herve; Graef, Claudia; Hornberger, Wilfried;
 Lange, Udo E. W.; Lauterbach, Arnulf; Seitz, Werner;
 Subkowski, Thomas

CORPORATE SOURCE: Discovery Research, Abbott GmbH and Co KG,
 Neuroscience, Medicinal Chemistry, Ludwigshafen,
 D-67008, Germany

SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(7),
 1319-1341

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

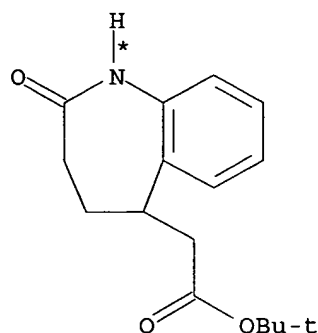
AB The design and synthesis of novel integrin $\alpha V\beta 3$ antagonists
 based on a 1,5- or 2,5-substituted tetrahydrobenzazepinone core is
 described. In vitro activity of resp. compds. was determined via
 $\alpha V\beta 3$ binding assay, and selected derivs. were submitted to
 further characterization in functional cellular assays. SAR was obtained
 by modification of the benzazepinone core, variation of the spacer linking
 guanidine moiety and core, and modification of the guanidine mimetic.
 These efforts led to the identification of novel $\alpha V\beta 3$
 inhibitors displaying potency in the subnanomolar range, selectivity vs.
 $\alpha IIb\beta 3$ and functional efficacy in relevant cellular assays. A
 method for the preparation of enantiomerically pure derivs. was developed, and
 resp. enantiomers evaluated in vitro. Compds. 31 and 37 were assessed for
 metabolic stability, resorption in the Caco-2 assay and pharmacokinetics.

RX(328) OF 714 COMPOSED OF REACTION SEQUENCE RX(3), RX(108)

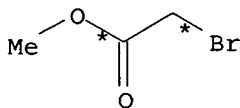
AND REACTION SEQUENCE RX(97), RX(12), RX(108)

...I + N ==> O...

... AN + O ==> CB

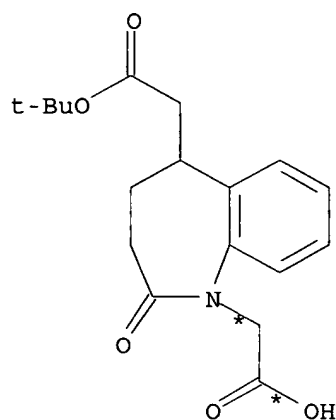


I



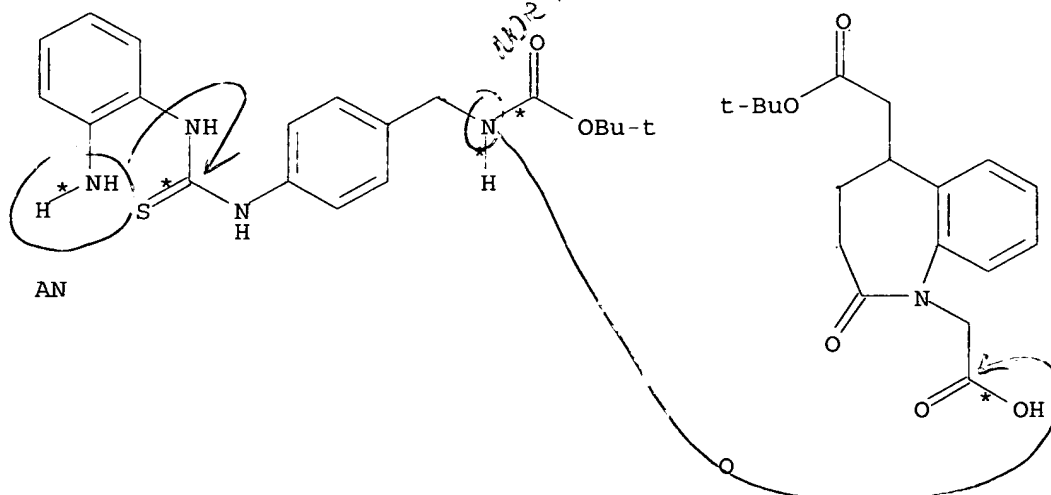
N

3
STEPS
→

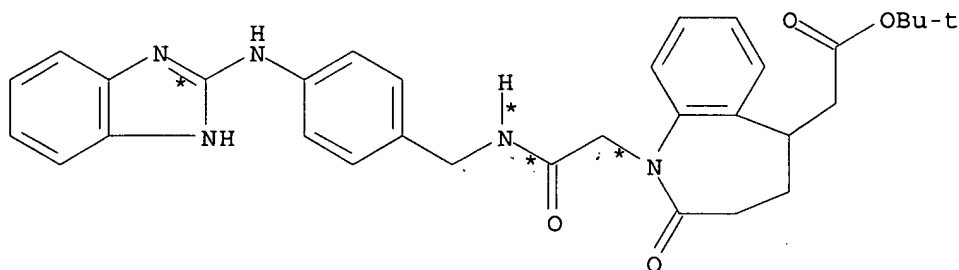


O

START NEXT REACTION SEQUENCE



3
STEPS
→



CB
YIELD 73%

RX(3) RCT I 380394-63-8

STAGE(1)

RGT C 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 10 - 20 deg C
SUBSTAGE(2) 1 hour, 10 - 20 deg C

STAGE(2)

RCT N 96-32-2
CON SUBSTAGE(1) 10 - 20 deg C
SUBSTAGE(2) 12 hours, 10 - 20 deg C

STAGE(3)

RGT P 1310-73-2 NaOH
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 45 minutes, room temperature

STAGE(4)

RGT Q 7646-93-7 KHSO4
SOL 7732-18-5 Water
CON room temperature, pH 7

PRO O 380394-64-9

RX(97) RCT AN 302341-66-8
RGT AZ 21908-53-2 HgO, BA 7704-34-9 S
PRO AQ 326410-47-3
SOL 64-17-5 EtOH
CON 2 hours, room temperature -> reflux

RX(12) RCT AQ 326410-47-3

RGT AJ 7647-01-0 HCl
PRO AR 570360-60-0
SOL 60-29-7 Et2O, 75-09-2 CH2Cl2
CON 2 hours, room temperature

RX(108) RCT O 380394-64-9, AR 570360-60-0

STAGE(1)

RGT CJ 109-02-4 N-Methylmorpholine
SOL 68-12-2 DMF
CON room temperature

STAGE(2)

RGT CK 136849-72-4 Methanaminium, N-[[[(1-cyano-2-ethoxy-2-oxoethylidene)amino]oxy] (dimethylamino)methylene]-N-methyl-, tetrafluoroborate(1-)
CON SUBSTAGE(1) 30 minutes, room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO CB 380396-14-5

REFERENCE COUNT: 71

THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 17 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:23452 CASREACT

TITLE: 2-Phenylamino-2-oxazolines from N-(2-hydroxyethyl)-N-phenylthioureas using TsCl/NaOH

AUTHOR(S): Na, Hye-Sun; Kim, Taek Hyeon

CORPORATE SOURCE: Department of Applied Chemistry and The Research Institute for Catalysis, Chonnam National University, Gwangju, 500-757, S. Korea

SOURCE: Journal of the Korean Chemical Society (2003), 47(6), 671-674

CODEN: JKCSEZ; ISSN: 1017-2548

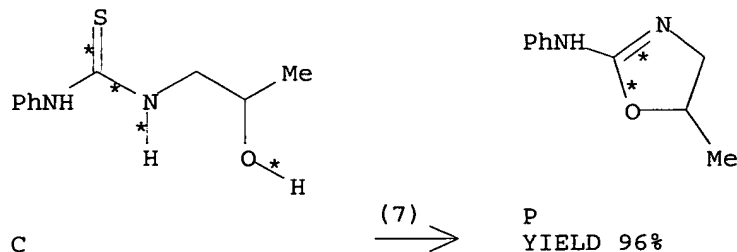
PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: Korean

AB Cyclization of N-(2-hydroxyethyl)-N-phenylthioureas with TsCl/NaOH in THF at room temperature for 30 min gave 2-phenylamino-2-oxazolines. For example, 4,5-dihydro-5-methyl-N-phenyl-2-oxazolamine was prepared in 96% yield from N-(2-hydroxypropyl)-N'-phenylthiourea.

RX(7) OF 18 ...C ==> P



RX(7) RCT C 29146-64-3

STAGE(1)

RGT Q 98-59-9 TsCl, R 1310-73-2 NaOH

SOL 7727-37-9 N2, 109-99-9 THF

CON 30 minutes, room temperature

STAGE(2)

RGT S 7732-18-5 Water

CON room temperature

PRO P 27151-02-6

L47 ANSWER 18 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:22185 CASREACT

TITLE: Synthesis of Some New Pyrido[4',3':4,5]thieno[2,3-d]pyrimidines and Related Fused Heterocycles

AUTHOR(S): Ahmed, Essam Kh.

CORPORATE SOURCE: Minia University, El-Minia, Egypt

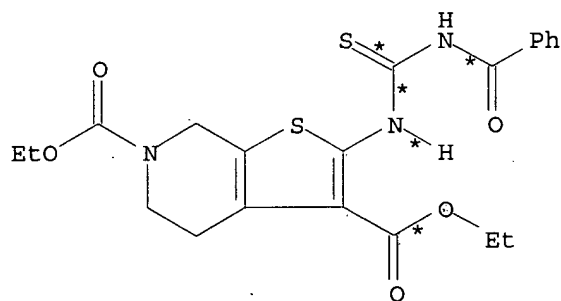
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2003), 178(1), 1-16
CODEN: PSSLEC; ISSN: 1042-6507

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

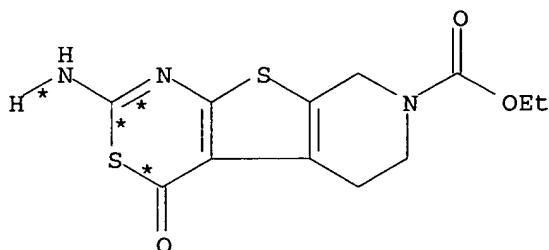
LANGUAGE: English

AB A highly efficient and versatile synthetic approach to the synthesis of pyrido[4',3':4,5]thieno[2,3-d]pyrimidines, pyrido[4',3':4,5]thieno[2,3-d][1,3]thiazolo[3,2-a]pyrimidines, pyrido[4'',3'':4',5']thieno[2',3':4,5]pyrimido[2,1-b][1,3]thiazine, and polymethylene condensed (e.g., pyrrolo-, piperidino-, azepino-)pyrido[4',3':4,5]thieno[2,3-d]pyrimidines is described utilizing di-Et 2-amino-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3,6-dicarboxylate as the starting material.

RX(2) OF 49 ...A ==> G

A

(2) →



G
YIELD 82%

RX(2) RCT A 538370-01-3

STAGE(1)

RGT H 7664-93-9 H₂SO₄
SOL 7732-18-5 Water
CON 2 days, room temperature

STAGE(2)

SOL 7732-18-5 Water
CON room temperature

STAGE(3)

RGT I 144-55-8 NaHCO₃
SOL 7732-18-5 Water
CON room temperature

PRO G 538370-02-4

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 19 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:151166 CASREACT

TITLE: Preparation of imidazoisoquinolinones as inhibitors of
tyrosine kinases

INVENTOR(S): Snow, Roger John; Cardozo, Mario; Goldberg, Daniel;
Hammach, Abdelhakim; Morwick, Tina; Moss, Neil; Patel,
Usha R.; Prokopowicz, Anthony S.; Takahashi, Hidenori;
Tschantz, Matt Aaron; Wang, Xiao-Jun

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 62 pp., Cont.-in-part of U.S.
Ser. No. 679,156.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002016460	A1	20020207	US 2001-921509	20010802

US 6506769 B2 20030114
 US 2003166929 A1 20030904
 US 6770639 B2 20040803

US 2002-292026 20021112

PRIORITY APPLN. INFO.:

US 1999-157922P 19991006
 US 2000-679156 20001005
 US 2001-921509 20010802

OTHER SOURCE(S): MARPAT 136:151166

AB The title compds. [I; Ar1 = (un)substituted (non)aromatic carbocyclyl, heteroaryl, heterocyclyl; X = NH, N(alkyl), O, etc.; Y = NR15, S, O; Ra = H, alkyl, alkenyl, etc.; R4 and R5 together with the atoms to which they are attached = II, III (wherein R6 = alkyl, H; R7 = alkyl, H; R8 = H, alkyl, etc.; R9 = H, CN, etc.)], useful as inhibitors of certain protein tyrosine kinases and are thus useful for treating diseases associated with such kinases, for example, diseases resulting from inappropriate cell proliferation, which include autoimmune diseases, chronic inflammatory diseases, allergic diseases, transplant rejection and cancer, as well as conditions resulting from cerebral ischemia, such as stroke, were prepared. All exemplified compds. I were evaluated in the tyrosine kinase assay using a kinase such as p56lck and were found to have IC50's less than 10 μ M. Methods of preparation are claimed and 29 example preps. are included. E.g., a multi-step synthesis of the imidazoisoquinolinedione IV was given. Claimed methods include: a method of making I wherein X is N-R15 and Ar1, R4, R5, R15 and Ra are as defined in claim 1, said process comprising: (a) reacting a phenylenediamine with Ar1NCS in a suitable solvent at about ambient to reflux temperature for .apprx.3 to 24 h to provide a possibly substituted N-(o-aminophenyl)thiourea (b) reacting this product with a suitable activating agent chosen from 1,3-dicyclohexylcarbodiimide (DCC) and mercuric oxide in a suitable solvent at about ambient to reflux temperature. Also, a method of making I wherein X is S, Y is NH and Ar1, R4, R5 and Ra are as defined in claim 1, said process comprising: (a) reacting an aniline with Ar1NCS in a suitable solvent at about ambient to reflux

temperature

for .apprx.3 to 24 h to form a thiourea; (b) reacting this product under cyclizing conditions in a suitable solvent at about reflux temperature. Also, a method of making V wherein R15, R8 and R9 are as described in claim 1, said method comprising: (a) reacting 2,6-dichloro-3-nitrobenzonitrile with NHR15 in a suitable solvent optionally in a pressure flask and at .apprx.0 to 80°, to provide 2-R15NH-3-nitro-6-chlorobenzonitriles, and subsequently reacting these compds. with ketoester R9C(O)CHR8CO2Et in the presence of a suitable base in a suitable solvent, at about ambient temperature to form 2-NC-3-R15NH-4-O2NC6H2CR8(C(O)R9)CO2Et (b) hydrolyzing this product by reacting with aqueous acid, and cyclizing at about reflux

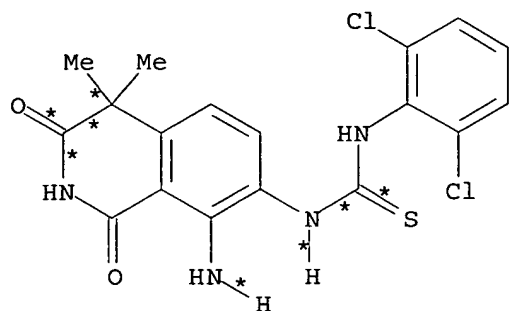
temperature;

followed by reducing the cyclized product in a suitable solvent. Also, a method of making VI wherein Ra, R8, R9 and Ar1 are as described in claim 1, said method comprising: (a) reacting a phenylenediamine with Br2 in a suitable solvent at ambient temperature to provide a brominated ring product; (b) reacting this product with Ar1NCS in a suitable solvent at about ambient to reflux temperature for .apprx.3 to 24 h and subsequently reacting

the

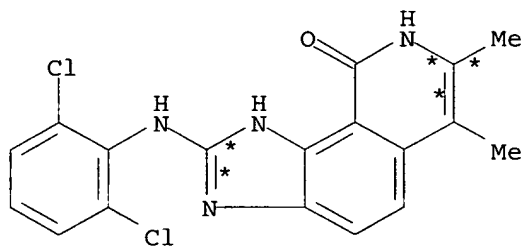
product with a suitable activating agent chosen from DCC and mercuric oxide in a suitable solvent at about ambient to reflux temperature to form VI with Ra = Br; (c) cross-coupling to introduce Ra in place of Br in the presence of a suitable catalyst in a suitable solvent at .apprx.100°.

RX(129) OF 348 COMPOSED OF RX(1), RX(35), RX(3)

RX(129) A ==> J

A

3
STEPS
→



J

YIELD 84%

RX(1) RCT A 333458-24-5
 RGT C 538-75-0 DCC
 PRO B 333455-06-4
 SOL 109-99-9 THF

RX(35) RCT B 333455-06-4

STAGE(1)

RGT G 16940-66-2 NaBH4
 CAT 7732-18-5 Water
 SOL 109-99-9 THF

STAGE(2)

RGT CO 7647-01-0 HCl
 SOL 7732-18-5 Water

STAGE(3)

RGT I 144-55-8 NaHCO3

PRO E 333458-25-6

RX(3) RCT E 333458-25-6

STAGE(1)

RGT K 7664-93-9 H2SO4
SOL 7664-93-9 H2SO4

STAGE(2)

RGT I 144-55-8 NaHCO3

PRO J 333455-11-1

L47 ANSWER 20 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:338107 CASREACT

TITLE: N-Acyl-4,5-dihydro-4,4-dimethyl-N-methyl-2-thiazolamine as a chemoselective acylating agent

AUTHOR(S): Kim, Taek Hyeon; Yang, Garp-Yeol

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National University, Gwangju, 500-757, S. Korea

SOURCE: Tetrahedron Letters (2002), 43(52), 9553-9557

CODEN: TELEAY; ISSN: 0040-4039

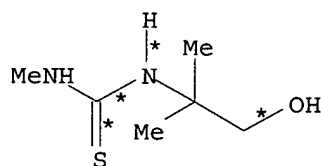
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

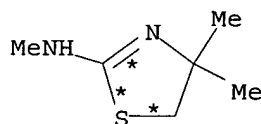
LANGUAGE: English

AB 4,5-Dihydro-N-methyl-2-thiazolamine and 4,5-dihydro-N,4,4-trimethyl-2-thiazolamine reacted with acyl halides to produce N-acyl-2-methylamino-2-thiazolines, (exo-acylated products) regioselectively; these were found to be highly chemoselective acylating agents for primary amine in the presence of secondary amine and for the less sterically hindered of two different primary amines. The N-acyldihydrothiazolamine acylation agents I (R = H, Me; R1 = Me, Et, tert-butyl) thus prepared included N-(4,5-dihydro-2-thiazolyl)-N-methylpropanamide, N-(4,5-dihydro-4,4-dimethyl-2-thiazolyl)-N-methylacetamide, N-(4,5-dihydro-4,4-dimethyl-2-thiazolyl)-N-methylpropanamide, and N-(4,5-dihydro-4,4-dimethyl-2-thiazolyl)-N,2,2-trimethylpropanamide.

RX(1) OF 47 A ==> B...



A



B
YIELD 83%

RX(1) RCT A 226989-34-0

STAGE(1)

RGT C 98-59-9 TsCl, D 1310-73-2 NaOH

SOL 109-99-9 THF, 7732-18-5 Water

CON SUBSTAGE(1) 5 minutes, room temperature

SUBSTAGE(2) 30 minutes, room temperature

STAGE(2)

RGT E 7732-18-5 Water
CON room temperature

PRO B 125101-37-3

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

22625

L47 ANSWER 21 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:194995 CASREACT

TITLE: Discovery of 2-Phenylamino-imidazo[4,5-h]isoquinolin-9-ones: A New Class of Inhibitors of Lck Kinase

AUTHOR(S): Snow, Roger J.; Cardozo, Mario G.; Morwick, Tina M.; Busacca, Carl A.; Dong, Yong; Eckner, Robert J.; Jacober, Stephen; Jakes, Scott; Kapadia, Suresh; Lukas, Susan; Panzenbeck, Maret; Peet, Gregory W.; Peterson, Jeffrey D.; Prokopowicz, Anthony S., III; Sellati, Rosemarie; Tolbert, Robert M.; Tschantz, Matt A.; Moss, Neil

CORPORATE SOURCE: Departments of Medicinal Chemistry, Chemical Development, Biology, Pharmacology, and Information Technology, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(16), 3394-3405

CODEN: JMCMAR; ISSN: 0022-2623

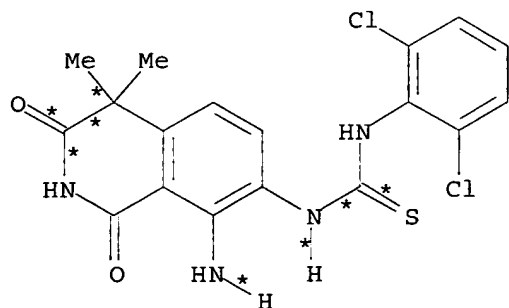
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

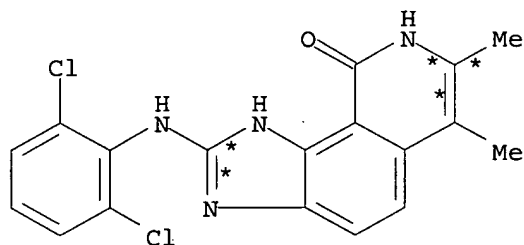
AB An imidazo[4,5-h]isoquinolin-7,9-dione (I) was identified as an ATP competitive inhibitor of lck by high throughput screening. Initial structure-activity relation studies identified the dichlorophenyl ring and the imide NH as important pharmacophores. A binding model was constructed to understand how I binds to a related kinase, hck. These results suggested that removing the gem-di-Me group and flattening the ring would enhance activity. This was realized by converting I to the imidazo[4,5-h]isoquinolin-9-one, resulting in an 18-fold improvement in potency against lck and a 50-fold increase in potency in a cellular assay.

RX(74) OF 222 COMPOSED OF RX(1), RX(13), RX(16)

RX(74) A ==> AS

A

3
STEPS
→



AS
YIELD 84%

RX(1) RCT A 333458-24-5
RGT C 538-75-0 DCC
PRO B 333455-06-4
SOL 109-99-9 THF

RX(13) RCT B 333455-06-4
RGT AN 16940-66-2 NaBH₄, K 7732-18-5 Water
PRO AM 333458-25-6
SOL 109-99-9 THF

RX(16) RCT AM 333458-25-6
RGT M 7664-93-9 H₂SO₄
PRO AS 333455-11-1

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 22 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:137075 CASREACT

TITLE: Synthesis and cyclic AMP phosphodiesterase 4 isoenzyme
inhibitory activity of heterocycle condensed purines
AUTHOR(S): Suzuki, Hirokazu; Yamamoto, Manabu; Shimura, Susumu;
Miyamoto, Ken-ichi; Yamamoto, Kenji; Sawanishi,
Hiroyuki

CORPORATE SOURCE: Department of Synthetic Chemistry, Hokuriku
University, Kanazawa, 920-1181, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(9),
1163-1168

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To reverse the adverse reactions of alkylxanthines and to develop novel
inhibitors of cAMP phosphodiesterase 4 (PDE4), a series of heterocycle
[a]-, [b]-, [c,d]-, and [i]-condensed purines were designed and
synthesized. Although all compds. did not display PDE1 and PDE3
inhibitory activities, several heterocycle [i]-condensed purines strongly
inhibited PDE4. Especially, dl-3,4-dipropyl-8-methyl-4,5,7,8-tetrahydro-1H-
imidazo[2,1-i]purin-5-one (I) exhibited comparable PDE4 inhibitory
activity (IC₅₀=1.9 μ M) to rolipram and denbufylline (DBF).

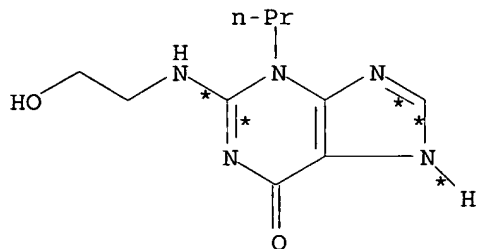
RX(62) OF 114 COMPOSED OF RX(7), RX(8), RX(19)

U

Z

AL

3
STEPS



RX (7) RCT U 492439-30-2

```
RGT  W 1310-73-2 NaOH
SOL  7732-18-5 Water
CON  SUBSTAGE(1) room temperature -> reflux
      SUBSTAGE(2) 3 hours, reflux
```

RGT X 7647-01-0 HCl
SOL 7732-18-5 Water

RX(8) RCT V 156733-29-8, Z 77-78-1

RGT W 1310-73-2 NaOH
SOL 7732-18-5 Water

CON 1 hour, room temperature

STAGE(2)

RGT AB 64-19-7 ACOH

PRO AA 492439-33-5

RX(19) RCT AA 492439-33-5, AL 141-43-5

PRO A 492439-59-5

SOL 110-86-1 Pyridine

CON overnight, reflux

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 23 OF 32 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:247890 CASREACT

TITLE: Enantioselective recognition of α -amino acid
derivatives with a cis-tetrahydrobenzoxanthene
receptor

AUTHOR(S): Oliva, Ana I.; Simon, Luis; Hernandez, Jose V.; Muniz,
Francisco M.; Lithgow, Anna; Jimenez, Alicia; Moran,
Joaquin R.

CORPORATE SOURCE: Departamento de Quimica Organica, Universidad de
Salamanca, Salamanca, E-37008, Spain

SOURCE: Journal of the Chemical Society, Perkin Transactions 2
(2002), (6), 1050-1052
CODEN: JCSPGI; ISSN: 1472-779X

PUBLISHER: Royal Society of Chemistry

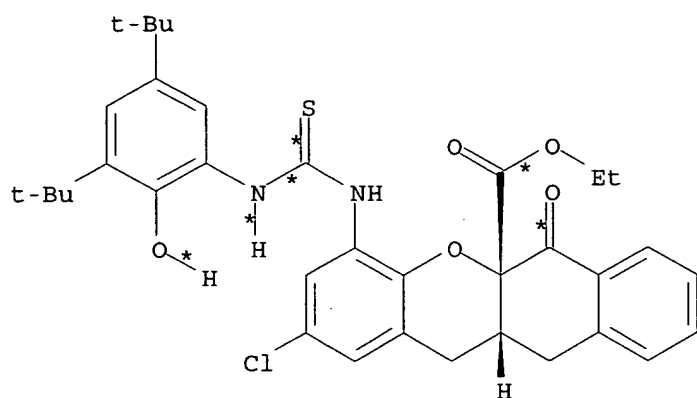
DOCUMENT TYPE: Journal

LANGUAGE: English

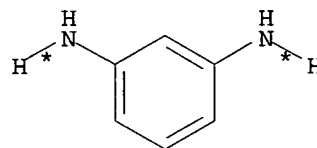
AB The synthesis of receptor I (R1 = OEt) was performed via oxidative
intramol. cyclization in several conventional synthetic steps, including
separation of trans isomer of racemic intermediate by crystallization, and its
structure was secured through X-ray diffraction anal. The
cis-tetrahydrobenzoxanthene receptor I (R1 = NH-mC6H5NHSO2CF3) was prepared
in high yield by transformation of receptor I (R1 = OEt). Competitive
1H-NMR titrns. were carried out by adding small amts. of the enantiomeric
pure guests (amino acid derivs.) to a deuteriochloroform solution of the
racemic host I (R1 = NH-mC6H5NHSO2CF3). Titration of guests revealed the
importance of the amino acid side chain and the carbamoyl substituent.
Benzyloxycarbonyl derivs. provide the best substrates, with chiral
recognitions of up to 15 (with Cbz-phenylglycine), while steric hindrance
from the tert-Bu group probably yields Boc derivs. with small association
consts. and poor enantioselectivities.

RX(21) OF 55 COMPOSED OF RX(9), RX(1), RX(10), RX(2)

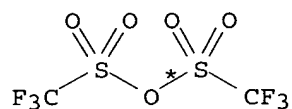
RX(21) AB + AF + F ==> G



AB

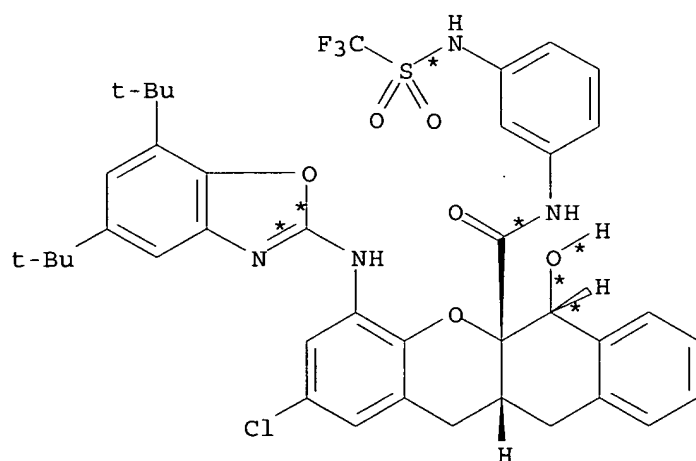


AF



F

4
STEPS
→



G
YIELD 88%

RX(9) RCT AB 460061-25-0
 RGT AC 74-88-4 MeI, AD 108-75-8 s-Collidine
 PRO A 460061-26-1
 SOL 64-17-5 EtOH, 109-99-9 THF

RX(1) RCT A 460061-26-1
 RGT C 54575-49-4 K Selectride
 PRO B 460061-19-2
 SOL 109-99-9 THF

RX(10) RCT B 460061-19-2, AF 240134-75-2
 PRO E 460061-27-2
 SOL 109-99-9 THF

RX(2) RCT E 460061-27-2, F 358-23-6
 PRO G 460061-20-5
 SOL 108-88-3 PhMe

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 24 OF 82 ~~CASREACT~~ ^{PRINTED} COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:103383 CASREACT

TITLE: Synthesis and SAR of N-substituted dibenzazepinone derivatives as novel potent and selective α V β 3 antagonists

AUTHOR(S): Kling, Andreas; Backfisch, Gisela; Delzer, Jurgen; Geneste, Herve; Graef, Claudia; Holzenkamp, Uta; Hornberger, Wilfried; Lange, Udo E. W.; Lauterbach, Arnulf; Mack, Helmut; Seitz, Werner; Subkowski, Thomas

CORPORATE SOURCE: Knoll GmbH, Ludwigshafen, D-67008, Germany

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(3), 441-446

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

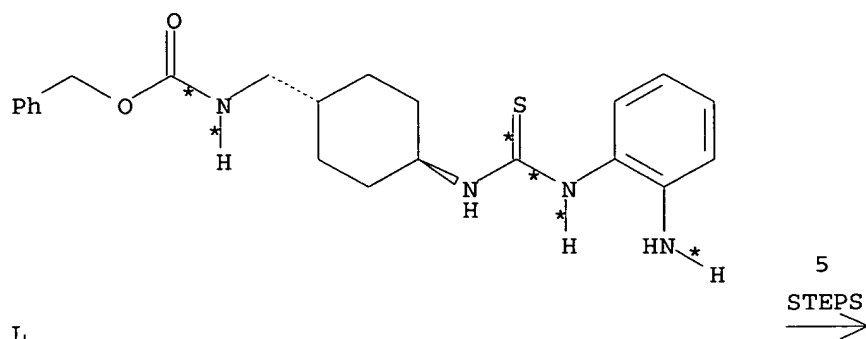
LANGUAGE: English

AB Substituted oxodibenzazepineacetic acids substituted with guanidines or guanidine pharmacophores such as I are prepared as potential α V β 3 (vitronectin receptor) antagonists. The oxodibenzazepineacetic acid core II is prepared in 5 steps from 9,10-anthraquinone; coupling of II with guanidine or guanidine pharmacophore-substituted amines such as III followed by hydrolysis of the Me ester yields compds. such as I. Structure-activity relationships are determined for the guanidine or guanidine pharmacophore-substituted oxodibenzazepineacetic acids, varying the linker between the guanidine pharmacophore and the oxodibenzazepine and the choice of guanidine pharmacophore. Compound I and a second guanidine pharmacophore-substituted oxodibenzazepineacetic acid are found to be highly active inhibitors of the vitronectin receptor in vitro and are found to be bioavailable in ADME assays.

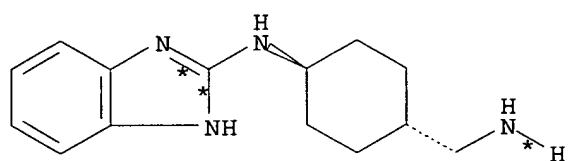
RX(295) OF 330 COMPOSED OF REACTION SEQUENCE RX(4), RX(5)
 AND REACTION SEQUENCE RX(6), RX(7), RX(8), RX(9), RX(5)

... L ==> O...

...Z + AE + AH + O ==> V



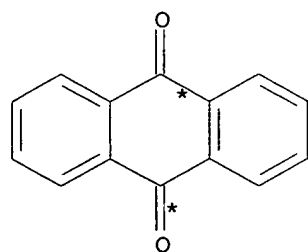
L



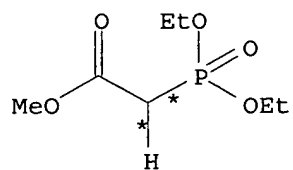
●2 HBr

O

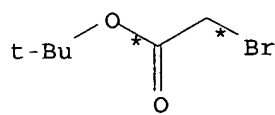
START NEXT REACTION SEQUENCE



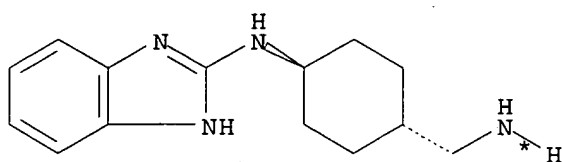
Z



AE



AH



● 2 HBr

5

STEPS
→

O

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT L 443330-59-4

STAGE(1)

RGT P 21908-53-2 HgO, Q 7704-34-9 S

SOL 64-17-5 EtOH

STAGE(2)

RGT R 10035-10-6 HBr

SOL 64-19-7 AcOH

PRO O 443330-62-9

NTE stereoselective

RX(6) RCT Z 84-65-1

RGT AB 26628-22-8 NaN₃, AC 7664-93-9 H₂SO₄

PRO AA 1143-50-6

SOL 7732-18-5 Water

RX(7) RCT AA 1143-50-6, AE 1067-74-9

RGT AG 7646-69-7 NaH

PRO AF 90664-74-7

SOL 68-12-2 DMF

RX(8) RCT AF 90664-74-7, AH 5292-43-3

RGT AG 7646-69-7 NaH

PRO AI 326404-40-4

SOL 68-12-2 DMF

RX(9) RCT AI 326404-40-4

STAGE(1)

RGT AJ 1333-74-0 H₂

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

STAGE(2)

RGT AK 76-05-1 F₃CCO₂HSOL 75-09-2 CH₂Cl₂

PRO U 326404-49-3
NTE high pressure in first stage

RX(5) RCT U 326404-49-3, O 443330-62-9
RGT W 25952-53-8 EDAP, X 7087-68-5 EtN(Pr-i)2
PRO V 443331-93-9
SOL 75-09-2 CH2Cl2, 68-12-2 DMF
NTE stereoselective

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 25 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:379462 CASREACT

TITLE: Biphenyls as potent vitronectin receptor antagonists

AUTHOR(S): Urbahns, Klaus; Harter, Michael; Albers, Markus;
Schmidt, Delf; Stelte-Ludwig, Beatrix; Bruggemeier,
Ulf; Vaupel, Andrea; Gerdes, Christoph

CORPORATE SOURCE: Pharma Research Centre, Institute of Medicinal
Chemistry, Bayer AG, Wuppertal, D-42096, Germany

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002),
12(2), 205-208

CODEN: BMCLE8; ISSN: 0960-894X

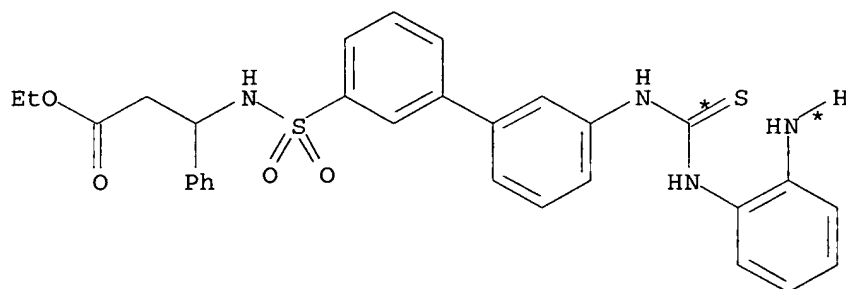
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

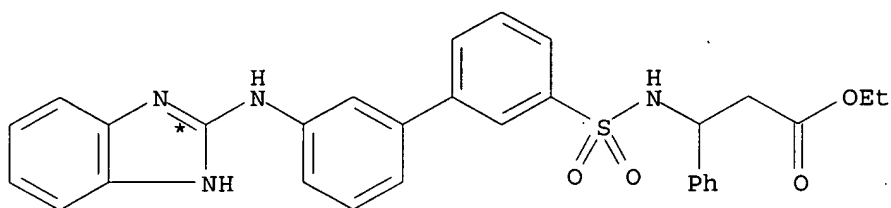
AB Vitronectin receptor ($\alpha V\beta 3$) antagonism has been implicated as a
mechanism for the treatment of restenosis following balloon angioplasty.
In this work the authors present results from screening of a focused
combinatorial library based on a biphenyl moiety. Our SAR studies led to
the identification of compds. with subnanomolar activity, selectivity
towards the related GPIIb/IIIa receptor and functional activity on human
smooth muscle cell migration.

RX(2) OF 13 ...D ==> G



D

(2) →



G

RX(2) RCT D 276258-86-7
 RGT H 21908-53-2 HgO
 PRO G 276258-87-8
 SOL 67-66-3 CHCl₃

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 26 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:271578 CASREACT

TITLE: Synthesis and antiinflammatory activity of novel 3-(2,3-dimethyl-1-phenyl-4-pyrazolon-5-yl)-4-thiazolidones

AUTHOR(S): Lesyk, R.; Vladzimirska, O.; Zimenkovsky, B.; Golota, S.; Nektgayev, I.; Cherpak, O.; Leb'yak, M.; Kozak, O.

CORPORATE SOURCE: Department of Pharmaceutical, Organic and Bioorganic Chemistry, Lviv State Medical University, Lviv-10, Ukraine

SOURCE: Bollettino Chimico Farmaceutico (2002), 141(3), 197-201

CODEN: BCFAAI; ISSN: 0006-6648

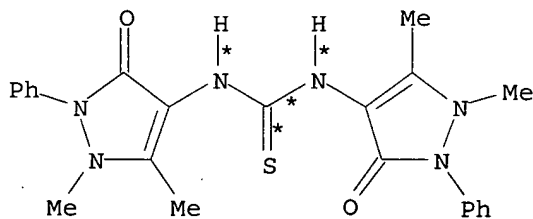
PUBLISHER: Societa Editoriale Farmaceutica

DOCUMENT TYPE: Journal

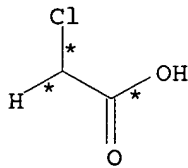
LANGUAGE: English

AB New 3-(2,3-dimethyl-1-phenyl-4-pyrazolon-5-yl)-4-thiazolidones were synthesized. The structure of substances was supported by UV- and ¹H-NMR spectra. Some compds. were tested in vivo for their anti-inflammatory activity. Previous results about structure-activity relationships were confirmed.

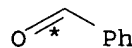
RX(2) OF 26 A + B + F ==> G...



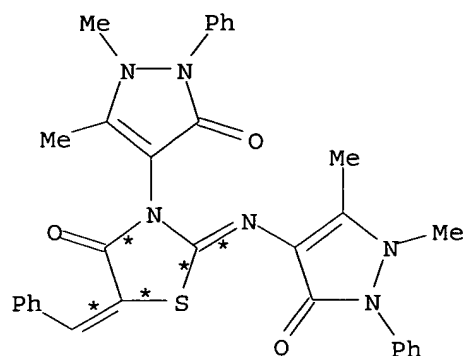
A



B



F

(2)
→

G
YIELD 61%

RX(2) RCT A 26084-35-5, B 79-11-8, F 100-52-7

STAGE(1)

RGT D 127-09-3 AcONa
SOL 64-19-7 AcOH
CON 7 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT H 7631-90-5 NaHSO₃
SOL 7732-18-5 Water

PRO G 314250-44-7

REFERENCE COUNT: 3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 27 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:6121 CASREACT

TITLE: Investigation of the cyclization of
N-(2-hydroxyethyl)-N'-phenylthioureas: Mitsunobu
conditions vs. TsCl/NaOH system

AUTHOR(S): Lee, Gue-Jae; Kim, Jae Nyoung; Kim, Taek Hyeon

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National
University, Kwangju, 500-757, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2002), 23(1),
19-20

CODEN: BKCSDE; ISSN: 0253-2964

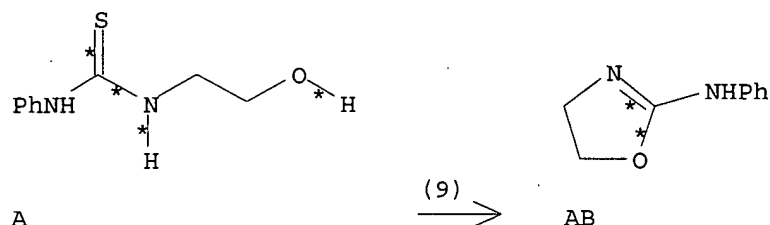
PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reaction of N-(2-hydroxyethyl)-N'-phenylthioureas under Mitsunobu conditions gave N- and S-cyclized products; in the TsCl/NaOH system 2-amino-2-oxazolines were formed via carbodiimide intermediates.

RX(9) OF 16 A ==> AB

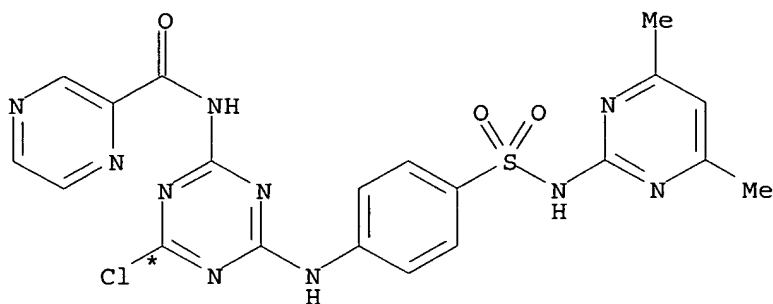


RX(9) RCT A 102-12-5
 RGT AC 98-59-9 TsCl, AD 1310-73-2 NaOH
 PRO AB 27151-01-5
 SOL 109-99-9 THF
 NTE regioselective

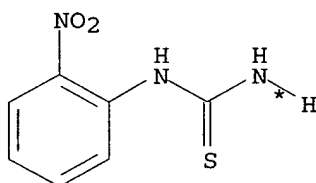
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 28 OF 82 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 141:140400 CASREACT
 TITLE: Antibacterial study of 2-(pyrazine-2'-carboxamido)-4-(2'-p-aminobenzene-sulfonamido-4', 6'-dimethyl pyrimidine)-6-(arylthioureido)-s-triazine derivatives
 AUTHOR(S): Patel, N. B.; Gorgamwala, Y. S.
 CORPORATE SOURCE: Department of Chemistry, South Gujarat University, Surat, 395007, India
 SOURCE: Journal of Indian Council of Chemists (2002), 19(2), 17-20
 CODEN: JICCE7; ISSN: 0971-5037
 PUBLISHER: Indian Council of Chemists
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 2-(Pyrazine-2'-carboxamido)-4-(2'-p-aminobenzene sulfonamido-4', 6'-dimethylpyrimidine)-6-(arylthioureido)-s-triazine derivs., e.g., I, have been synthesized from 2-(pyrazine-2'-carboxamido)-4-(2'-p-aminobenzene sulfonamido-4', 6'-dimethyl pyrimidine)-6-chloro-s-triazine via 2-(pyrazine-2'-carboxamido)-4, 6-dichloro-triazine and have been screened for antibacterial strain against S. aureus & E. coli. Among them, I, II, and III show significant antibacterial activity.

RX(5) OF 33 ...A + K ==> L



A



K



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX (5) RCT A 726172-39-0, K 51039-84-0
 PRO L 726172-33-4
 SOL 67-64-1 Me2CO
 CON 3 hours, reflux

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 29 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 137:169447 CASREACT

TITLE: L-Valinol and L-phenylalaninol-derived
 2-phenylamino-2-oxazolines as chiral auxiliaries in
 asymmetric alkylations

AUTHOR(S): Lee, Gue-Jae; Kim, Taek Hyeon; Kim, Jae Nyoung; Lee,
 Uk

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National
 University, Kwangju, 500-757, S. Korea

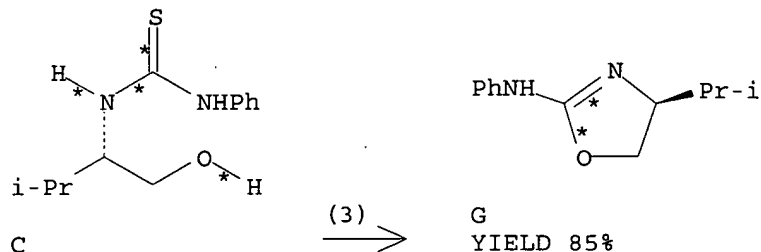
SOURCE: Tetrahedron: Asymmetry (2002), 13(1), 9-12
 CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Lithium enolates of N-acyl-2-phenyliminooxazolidine auxiliaries reacted with alkyl halides to produce the α -alkylated products with very high diastereofacial selectivity (up to >99% d.e.). The products were readily cleaved by simple alkaline hydrolysis to give homochiral carboxylic acids and could also be directly converted to aldehydes and other acid derivs. such as esters and amides.

RX(3) OF 56 ... C ==> G...

RX(3) RCT C 254900-23-7
 RGT H 98-59-9 TsCl, I 1310-73-2 NaOH
 PRO G 236386-37-1
 SOL 109-99-9 THF
 NTE stereoselective

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓ L47 ANSWER 30 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:331378 CASREACT

TITLE: A mild cyclodesulfurization of N-(2-hydroxyethyl)-N'-phenylthioureas to 2-phenylamino-2-oxazolines using TsCl/NaOH

AUTHOR(S): Kim, T. H.; Lee, N.; Lee, G.-J.; Kim, J. N.

CORPORATE SOURCE: College of Engineering, Faculty of Applied Chemistry, Chonnam National University, Kwangju, 500-757, S. Korea

SOURCE: Tetrahedron (2001), 57(33), 7137-7141

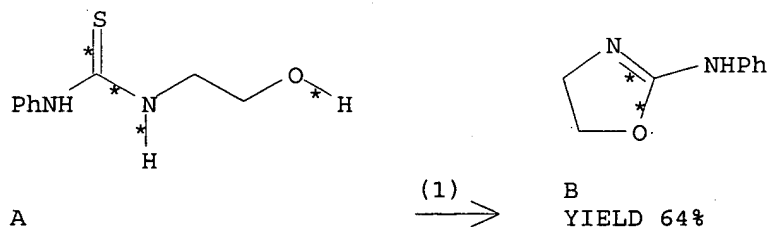
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An efficient synthesis of 2-phenylamino-2-oxazolines via cyclodesulfurization of N-(2-hydroxyethyl)-N'-phenylthioureas by a one-pot reaction using p-toluenesulfonyl chloride (TsCl) and NaOH in very good yields is described.

RX(1) OF 12 A ==> B

RX(1) RCT A 102-12-5

STAGE(1)

RGT C 1310-73-2 NaOH, D 98-59-9 TsCl

SOL 109-99-9 THF, 7732-18-5 Water

STAGE(2)

RGT E 7732-18-5 Water

PRO B 27151-01-5

NTE regioselective, alternative reaction conditions shown

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 31 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:344680 CASREACT

TITLE: trans-Benzoxanthene receptors for enantioselective
recognition of amino acid derivativesAUTHOR(S): Perez, Emilio M.; Oliva, Ana I.; Hernandez, Jose V.;
Simon, Luis; Moran, Joaquin R.; Sanz, FranciscaCORPORATE SOURCE: Departamento de Quimica Organica, Universidad de
Salamanca, Salamanca, E-37008, Spain

SOURCE: Tetrahedron Letters (2001), 42(34), 5853-5856

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

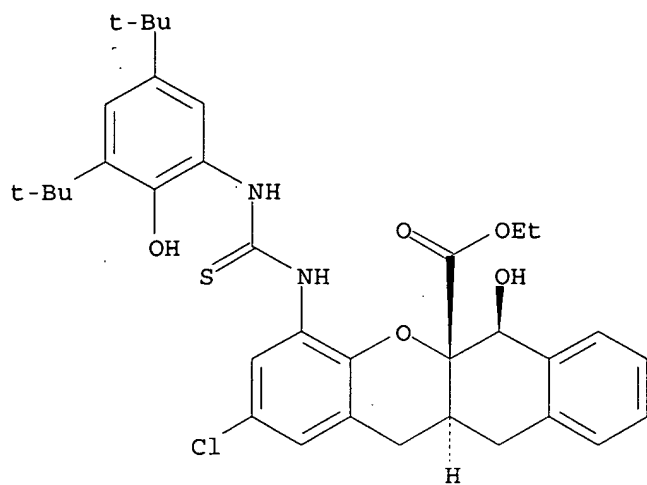
DOCUMENT TYPE: Journal

LANGUAGE: English

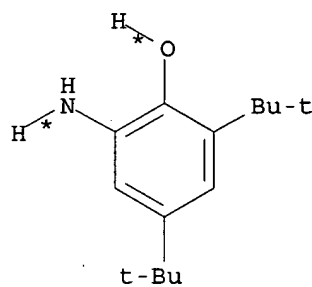
AB Neutral cleft-type hydrogen-bonding receptors (I) based on a
trans-benzoxanthene skeleton have shown good stereoselective association
towards carbamate derivs. of amino acids. Among these, the best results
corresponded to the com. available benzyloxycarbamate (Cbz) while the
t-butyloxycarbamate (Boc) protecting group afforded disappointing results.
Preparative TLC impregnated in ethoxycarbonyl proline provided a rapid way
to resolve the receptor racemic mixture X-Ray anal. and Overhauser effects
allow us to suggest a structure for these complexes and the reasons for
the observed chiral discrimination.

RX(29) OF 45 COMPOSED OF RX(7), RX(8), RX(9)

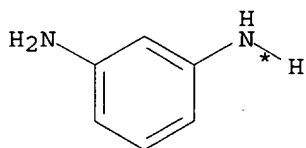
RX(29) T + S + AA + AD ==> AE



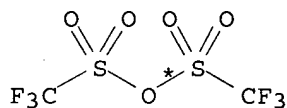
T



S

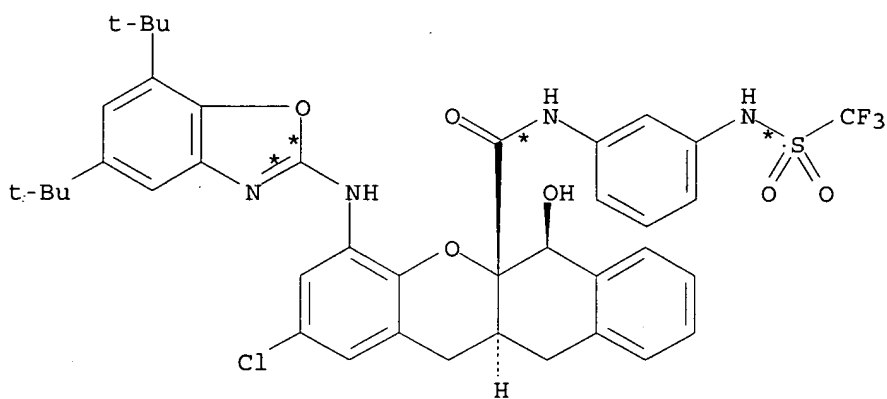


AA



AD

3
STEPS
→



AE

YIELD 63%

RX(7)

RCT T 370862-26-3, S 1643-39-6

RGT W 74-88-4 MeI, X 108-75-8 s-Collidine

PRO V 370862-18-3

SOL 64-17-5 EtOH, 109-99-9 THF

RX(8) RCT V 370862-18-3, AA 108-45-2
 RGT AC 109-72-8 BuLi
 PRO AB 370862-27-4
 SOL 109-99-9 THF

RX(9) RCT AB 370862-27-4, AD 358-23-6
 PRO AE 370862-28-5
 SOL 108-88-3 PhMe

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 32 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:344423 CASREACT

TITLE: Cyclization of N-(2-hydroxyethyl)-N-phenylmethyl-N'-substituted ureas and thioureas: prelude to the synthesis of 1-aryl-substituted 2-imidazolidinones on solid support

AUTHOR(S): Kim, Taek Hyeon; Lee, Namgun; Kim, Jae Nyoung

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National University, Kwangju, 500-757, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2001), 22(7), 761-764

CODEN: BKCSDE; ISSN: 0253-2964

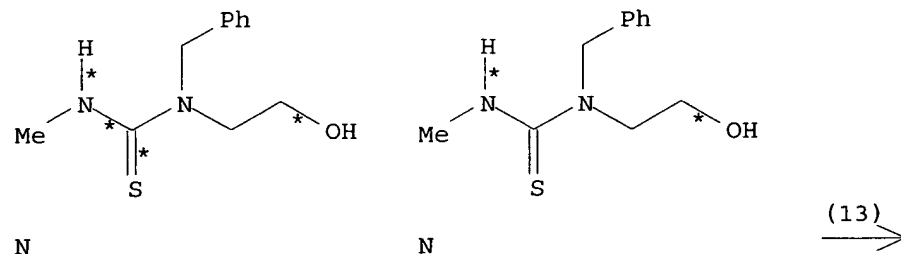
PUBLISHER: Korean Chemical Society

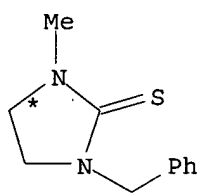
DOCUMENT TYPE: Journal

LANGUAGE: English

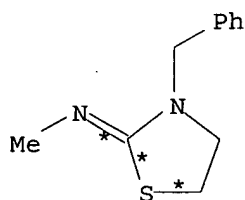
AB Ureas prepared in this study included: N'-ethyl-N-(2-hydroxyethyl)-N-(phenylmethyl)urea, N-(2-hydroxyethyl)-N'-phenyl-N-(phenylmethyl)urea, N-(2-Hydroxyethyl)-N'-(4-nitrophenyl)-N-(phenylmethyl)urea, N'-benzoyl-N-(2-hydroxyethyl)-N-(phenylmethyl)urea, etc. Thioureas prepared included N'-benzoyl-N-(2-hydroxyethyl)-N-(phenylmethyl)thiourea, N-(2-hydroxyethyl)-N'-phenyl-N-(phenylmethyl)thiourea and N-(2-hydroxyethyl)-N'-methyl-N-(phenylmethyl)thiourea. Cyclization of these urea and thiourea intermediates gave imidazolidinones and imidazolidinethiones.

RX(13) OF 24 ...2 N ==> AA + AB





AA
YIELD 18%



AB
YIELD 35%

RX(13) RCT N 370553-03-0
RGT T 1310-73-2 NaOH, U 98-59-9 TsCl
PRO AA 370553-05-2, AB 370553-04-1
SOL 109-99-9 THF, 7732-18-5 Water
NTE alternative preparation shown

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 33 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:5550 CASREACT

TITLE: Cyclization reaction of N-(2-hydroxyethyl)-N'-methylthioureas in the presence of TsCl and base

AUTHOR(S): Lee, Namgun; Cha, Mi-Hyun; Kim, Taek Hyeon

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National University, Kwangju, 500-757, S. Korea

SOURCE: Journal of the Korean Chemical Society (2001), 45(1), 96-99

CODEN: JKCSEZ; ISSN: 1017-2548

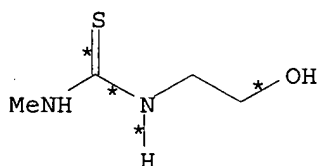
PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Thioureas I (R1 = H, Me, Et, PhCH₂; R2 = H, Me; R3 = H, Et), prepared by condensation of aminoalcs. with MeNCS, were conveniently converted under one-pot reaction conditions using t-BuOK and TsCl into iminothiazolidines II (R3 = H, Me, Et) and imidazolethiones III (R3 = Me, Et).

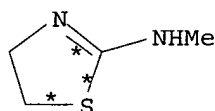
RX(8) OF 25 ...C ==> Q



C



Q



RX(8) RCT C 3120-26-1

RGT R 98-59-9 TsCl, S 121-44-8 Et3N, T 1122-58-3 4-DMAPPRO Q 10416-51-0

SOL 109-99-9 THF

NTE regioselective, alternative prepn. shown

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 34 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:57786 CASREACT

TITLE: Potential of pyrazolooxadiazinone derivatives as serine protease inhibitors

AUTHOR(S): Vicentini, C. B.; Guarneri, M.; Andrisano, V.; Guccione, S.; Langer, T.; Marschhofer, R.; Chabin, R.; Edison, A. M.; Huang, X.; Knight, W. B.; Giori, P.

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Ferrara, Italy

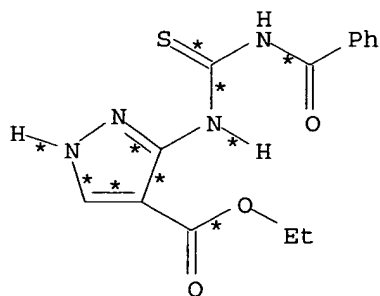
SOURCE: Journal of Enzyme Inhibition (2001), 16(1), 15-34
CODEN: ENINEG; ISSN: 8755-5093

PUBLISHER: Harwood Academic Publishers

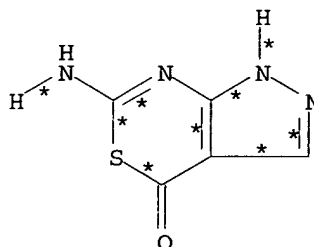
DOCUMENT TYPE: Journal

LANGUAGE: English

AB As a part of an investigation on mol. hybrids as new serine protease inhibitors, the pyrazolo [4,3-c] [1,2,5]oxadiazin-3(5H)-one ring system was selected as a model of potential mechanism-based inhibitors. Due to the inherent reactivity of this system an optimal balance between susceptibility to nucleophilic attack and stability in solvents was sought prior to development as therapeutic agents. Substitutions on N5 and C7 of the supporting pyrazole ring with either aliphatic or aromatic groups and the replacement of the carbonyl oxygen on the reactive oxadiazinone ring with sulfur were explored. Two members of this class of inhibitors displayed time-dependent inhibition of human leukocyte elastase (HLE) suggesting mechanism-based inhibition. The observation that HLE generated a product(s) which displayed an identical UV-Visible spectrum to that observed during non-enzymic hydrolysis further supports this proposal. FlexX-based docking of these compds. into a model of HLE active site produced a mol. model of the inhibitor-enzyme interaction.

RX(15) OF 32 ...AG ==> AK

AG



AK
YIELD 80%

RX(15) RGT AG 138480-76-9

STAGE(1)

RGT AL 7664-93-9 H2SO4

STAGE(2)

SOL 7732-18-5 Water

PRO AK 345633-64-9

REFERENCE COUNT: 50

THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L47 ANSWER 35 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 134:56618 CASREACT

TITLE: Modified Guanidines as Potential Chiral Superbases. 3.
Preparation of 1,4,6-Triazabicyclooctene Systems and
1,4-Disubstituted 2-Iminoimidazolidines by the
2-Chloro-1,3-dimethylimidazolinium Chloride-Induced
Cyclization of Guanidines with a Hydroxyethyl
SubstituentAUTHOR(S): Isobe, Toshio; Fukuda, Keiko; Yamaguchi, Kentaro;
Seki, Hiroko; Tokunaga, Tatsuhiko; Ishikawa, TsutomuCORPORATE SOURCE: Faculty of Pharmaceutical Sciences and Chemical
Analysis Center, Chiba University, Inage Chiba,
263-8522, JapanSOURCE: Journal of Organic Chemistry (2000), 65(23), 7779-7785
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

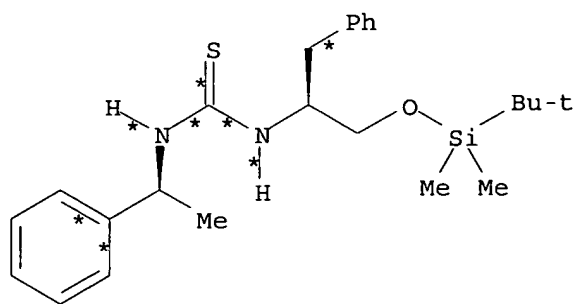
DOCUMENT TYPE: Journal

LANGUAGE: English

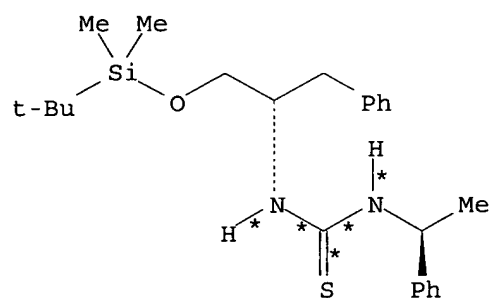
AB Simple preparation methods of modified guanidines have been explored as potential chiral superbases. Thus, 3,7,8-trisubstituted and 3,6,7,8-tetrasubstituted 1,4,6-triazabicyclooctene systems were prepared from (1S,2S)-1,2-diphenylethylenediamine through stepwise 2-chloro-1,3-dimethylimidazolinium chloride (DMC)-induced cyclizations of protected thioureas to the corresponding 2-iminoimidazolidines and then of 2-(2-hydroxyethylimino)imidazolidines to the bicyclic systems.. Linear guanidines with a 2-hydroxyethyl functional group were prepared by the reaction of carbodiimides with 2-amino alcs. Reaction of linear-type guanidines with DMC followed by base treatment afforded 1,4-disubstituted 2-iminoimidazolidines. Furthermore, another type of 1,4,6-triazabicyclooctene was also prepared through double DMC-induced cyclization of guanidines with two 2-hydroxyethyl substituents.

RX(126) OF 186 COMPOSED OF RX(40), RX(33), RX(34)

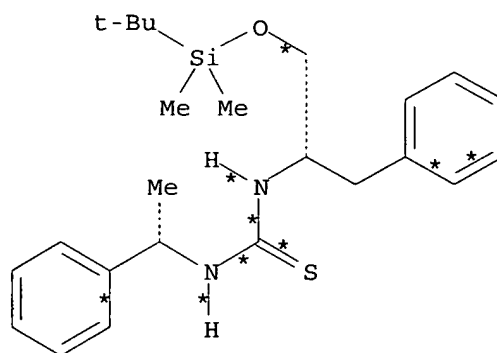
RX(126) 3 BV + 3 A ==> BL + BM + BN



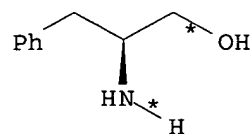
BV



BV

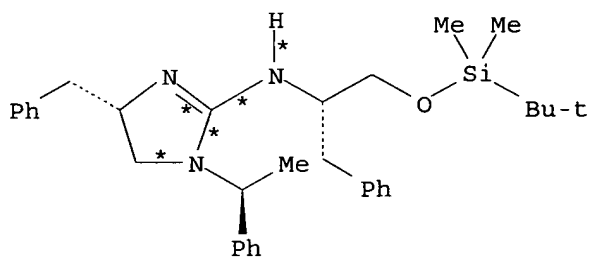


BV

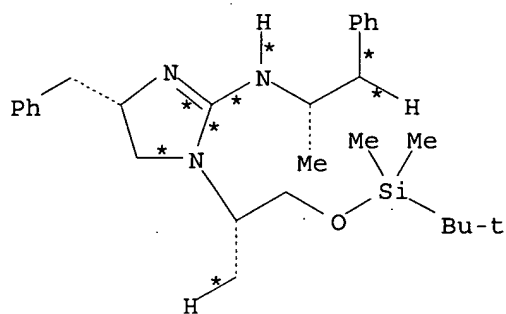


3 A

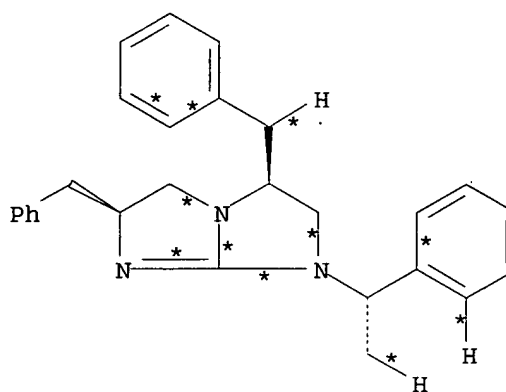
3
STEPS
→



BL



BM



BN

YIELD 15%

RX(40) RCT BV 314050-81-2
 RGT D 121-44-8 Et3N, K 37091-73-9 1H-Imidazolium, 2-chloro-4,5-dihydro-1,3-dimethyl-, chloride
 PRO BJ 314050-82-3
 SOL 75-09-2 CH2Cl2

RX(33) RCT BJ 314050-82-3, A 3182-95-4
 PRO BK 314050-73-2
 SOL 108-88-3 PhMe

RX(34) RCT BK 314050-73-2

STAGE(1)

RGT BO 75-75-2 MeSO3H

STAGE(2)

RGT K 37091-73-9 1H-Imidazolium, 2-chloro-4,5-dihydro-1,3-dimethyl-, chloride, D 121-44-8 Et3N

SOL 75-09-2 CH2Cl2

STAGE(3)

RGT AS 1310-58-3 KOH

SOL 67-56-1 MeOH

PRO BL 314050-74-3, BM 314050-79-8, BN 314050-75-4

NTE 94% overall yield

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 36 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 133:17720 CASREACT

TITLE: Synthesis of 2-Substituted Polyhydroxytetrahydropyrimidines (N-Hydroxy Cyclic Guanidino-Sugars): Transition-State Mimics of Enzymatic Glycosidic Cleavage

AUTHOR(S): Le, Van-Duc; Wong, Chi-Huey

CORPORATE SOURCE: Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Journal of Organic Chemistry (2000), 65(8), 2399-2409
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

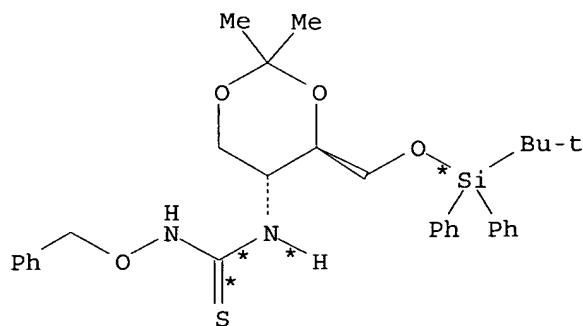
LANGUAGE: English

AB The synthesis of 2-substituted polyhydroxytetrahydropyrimidines as transition-state mimics of enzymic glycosidic cleavage has been achieved by using guanylation and cyclization methodologies. The D-galacto type N-hydroxy cyclic guanidino-sugar was synthesized in six steps from an amine and thiourea in an overall yield of 59%. To further derivatize this compound to incorporate the leaving group moiety, we have synthesized 2-methylsulfanyl compds. as key intermediates. The 2-methylsulfanyl group was displaced with amines, assisted by silver tetrafluoroborate as Lewis acid, to give protected cyclic guanidines in moderate yields (60-67%). Removal of the protecting groups gave the D-galacto-type N-hydroxy cyclic guanidino-sugar. The key steps in the synthesis of the 6-deoxy-DL-galacto type N-hydroxy cyclic guanidino-sugars involve cyclization of the appropriate acetal intermediates followed by removal of the protecting groups. A preliminary biol. evaluation on some of the final products showed no inhibitory activity against α - or β -galactosidase but some moderate activity against α -fucosidase.

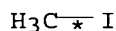
*1:2 enantiomers
(competing
reactions?)*

RX(159) OF 183 COMPOSED OF RX(14), RX(15), RX(16), RX(20), RX(21)

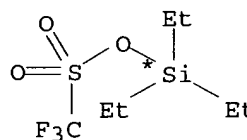
RX(159) I + AP + AF + E ==> BB



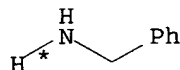
I



AP

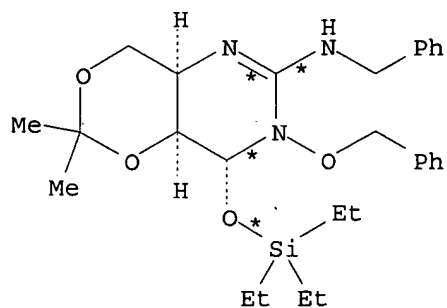


AF



E

5
STEPS
→



BB

YIELD 67%

RX(14) RCT I 272106-63-5

STAGE(1)

RGT AR 7646-69-7 NaH

SOL 64-17-5 EtOH

STAGE(2)

RCT AP 74-88-4

STAGE(3)

SOL 7732-18-5 Water

STAGE(4)

SOL 141-78-6 AcOEt

PRO AQ 272106-64-6

NTE STEREOSELECTIVE

RX(15) RCT AQ 272106-64-6

STAGE(1)

RGT R 429-41-4 Bu₄N.F

SOL 109-99-9 THF

STAGE(2)

SOL 141-78-6 AcOEt

PRO AT 272106-65-7

NTE STEREOSELECTIVE

RX(16) RCT AT 272106-65-7

STAGE(1)

RGT AB 87413-09-0 Martin's reagent

SOL 75-09-2 CH₂Cl₂

STAGE(2)

SOL 141-78-6 AcOEt

STAGE(3)

SOL 7732-18-5 Water

PRO AU 272106-66-8
NTE STEREOSELECTIVE

RX(20) RCT AU 272106-66-8, AF 79271-56-0

STAGE(1)
RGT AH 108-48-5 2,6-Lutidine
SOL 75-09-2 CH₂Cl₂

STAGE(2)
SOL 141-78-6 AcOEt

PRO BA 272106-70-4
NTE STEREOSELECTIVE

RX(21) RCT BA 272106-70-4, E 100-46-9

STAGE(1)
RGT BC 14104-20-2 AgBF₄, M 121-44-8 Et₃N
SOL 75-05-8 MeCN

STAGE(2)
SOL 141-78-6 AcOEt

PRO BB 272106-71-5
NTE STEREOSELECTIVE

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 37 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 134:29346 CASREACT

TITLE: Ring closure of N-(2-hydroxyethyl)-N'-phenylthioureas:
one-pot synthesis of 2-(phenylamino)thiazolines

AUTHOR(S): Kim, Taek Hyeon; Min, Jung Ki; Lee, Gue-Jae

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National
University, Kwangju, 500-757, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2000), 21(9),
919-922

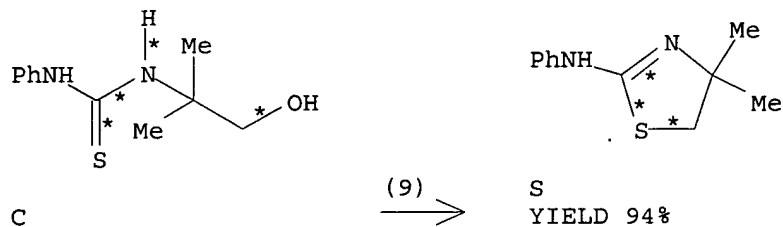
CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The cyclization reaction of N-(2-hydroxyethyl)-N'-phenylthioureas containing an ambident nucleophile was examined with a variety of bases plus p-toluenesulfonyl chloride (TsCl). N-(2-Hydroxyethyl)thioureas were readily obtained in high yields from the reaction of the corresponding 2-aminoalkanols with Ph isothiocyanate, avoiding the need for O-protection. The use of a one-pot reaction (NaOH/TsCl) was found to be most effective in producing the requisite 2-(phenylamino)thiazolines (S-cyclization) in the case of thioureas derived from N-unsubstituted amino alcs., while for thioureas prepared from N-substituted amino alcs. the combination of Et₃N and TsCl led to the S-cyclization products.

RX(9) OF 22 ...C ==> S

RX(9) RCT C 2654-06-0
 RGT T 98-59-9 TsCl, U 1310-73-2 NaOH
 PRO S 5744-31-0
 SOL 7732-18-5 Water, 109-99-9 THF

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 38 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:93244 CASREACT

TITLE: One-pot synthesis of 2-(phenylamino)thiazolines from N-(2-hydroxyethyl)-N'-phenylthioureas

AUTHOR(S): Kim, Taek Hyeon; Min, Jung Ki; Lee, Gue-Jae

CORPORATE SOURCE: Faculty of Applied Chemistry, Chonnam National University, Kwangju, 500-757, S. Korea

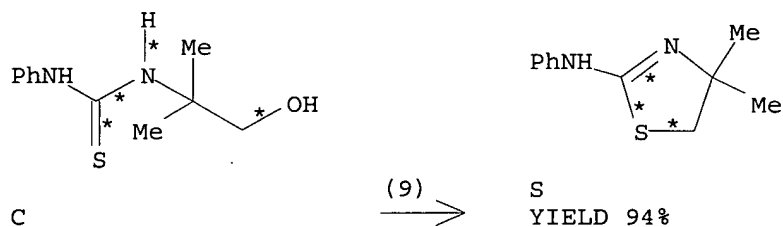
SOURCE: Tetrahedron Letters (1999), 40(47), 8201-8204
 CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 2-(Phenylamino)thiazolines were synthesized from N-(2-hydroxyethyl)-N'-phenylthioureas and PhNCS by a 1-pot reaction using 4-tosyl chloride and NaOH or Et₃N.

RX(9) OF 22 ...C ==> S

RX(9) RCT C 2654-06-0

STAGE(1)

RGT T 98-59-9 TsCl, U 1310-73-2 NaOH

SOL 109-99-9 THF

STAGE(2)
SOL 7732-18-5 Water

STAGE(3)
SOL 60-29-7 Et2O

PRO S 5744-31-0

REFERENCE COUNT: 14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 39 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:151751 CASREACT

TITLE: 2-(Diethylamino)thieno[1,3]oxazin-4-ones as Stable
Inhibitors of Human Leukocyte Elastase

AUTHOR(S): Guetschow, Michael; Kuerschner, Lars; Neumann, Ulf;
Pietsch, Markus; Loeser, Reik; Koglin, Norman; Eger,
Kurt

CORPORATE SOURCE: Institute of Pharmacy, University of Leipzig, Leipzig,
D-04103, Germany

SOURCE: Journal of Medicinal Chemistry (1999), 42(26),
5437-5447

CODEN: JMCMAR; ISSN: 0022-2623

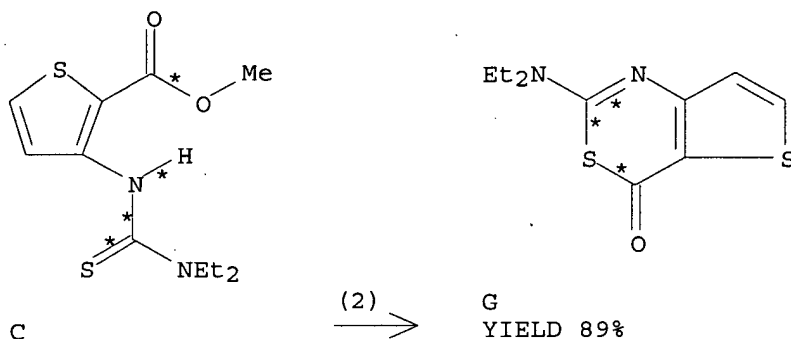
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 2-(diethylamino)thieno[1,3]oxazin-4-ones was synthesized and evaluated in vitro for inhibitory activity toward human leukocyte elastase (HLE). The Gewald thiophene synthesis was utilized to obtain several 2-aminothiophene-3-carboxylates. These precursors were subjected to a 5-step route to obtain thieno[2,3-d][1,3]oxazin-4-ones bearing various substituents at positions 5 and 6. Both thieno[2,3-d]- and thieno[3,2-d]-fused oxazin-4-ones possess extraordinary chemical stability, which was expressed as rate consts. of the alkaline hydrolysis. The kinetic parameters of the HLE inhibition were determined. The most potent compound, 2-(diethylamino)-4H-[1]benzothieno[2,3-d][1,3]oxazin-4-one, exhibited a K_i value of 5.8 nM. 2-(Diethylamino)thieno[1,3]oxazin-4-ones act as acyl-enzyme inhibitors of HLE, similar to the inhibition of serine proteases by 4H-3,1-benzoxazin-4-ones. The isosteric benzene-thiophene replacement accounts for an enhanced stability of the acyl-enzyme intermediates.

RX(2) OF 35 ...C ==> G...



RX(2) RCT C 257610-82-5

STAGE(1)

RGT H 7664-93-9 H₂SO₄

STAGE(2)

SOL 7732-18-5 Water

PRO G 257610-83-6

REFERENCE COUNT: 75

THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 40 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:151753 CASREACT

TITLE: Comment on cyclization of 2-(3-benzoylthioureido)benzonitrile in sulfuric acid

AUTHOR(S): Pazdera, Pavel; Sibor, Jiri

CORPORATE SOURCE: Department of Organic Chemistry, Faculty of Sciences, Masaryk University, Brno, CZ-611 37, Czech Rep.

SOURCE: Scripta--Chemistry (1998), Volume Date 1997-1998, 27-28, 27-32

CODEN: SCCHEB; ISSN: 1210-8456

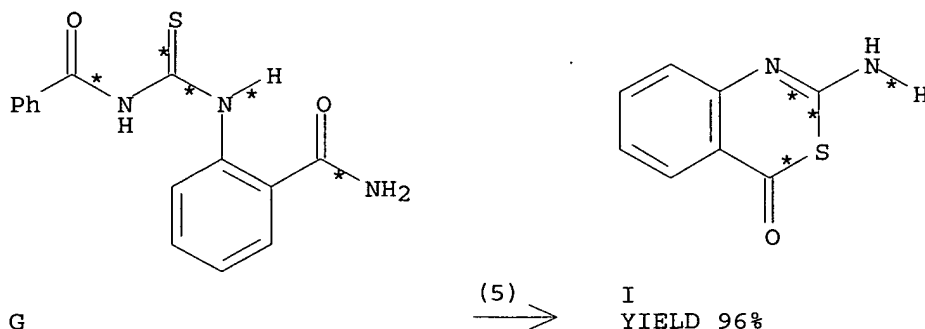
PUBLISHER: Masarykova Universita v Brne, Prirodovedecka Fakulta

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Cyclization of 2-(3-benzoylthioureido)benzonitrile by action of sulfuric acid is reported. The main product, i.e. 2-benzoylamino-4-imino-4H-3,1-benzothiazine (I), is formed directly. 2-(3-Benzoylthioureido)benzamide, 2-benzoylamino-4H-3,1-benzothiazine-4-one, and 2-amino-4H-3,1-benzothiazine-4-one were obtained from I during consequent reactions.

RX(5) OF 6 ...G ==> I



RX(5) RCT G 115934-14-0
 RGT C 7664-93-9 H₂SO₄
 PRO I 131357-73-8
 SOL 7732-18-5 Water

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

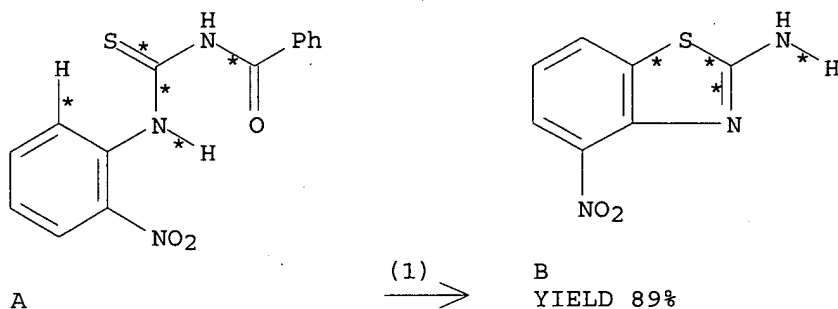
L47 ANSWER 41 OF 82 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 125:275861 CASREACT
 TITLE: Preparation of 2-aminobenzothiazoles
 INVENTOR(S): Malinowski, Wlodzimierz; Szadowski, Jerzy; Kraska, Jan
 PATENT ASSIGNEE(S): Politechnika Lodzka, Pol.
 SOURCE: Pol., 3 pp.
 CODEN: POXXA7
 DOCUMENT TYPE: Patent
 LANGUAGE: Polish
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PL 165691	B1	19950131	PL 1991-292770	19911212

PRIORITY APPLN. INFO.: PL 1991-292770 19911212

AB The title mono-, di- and trisubstituted 2-aminobenzothiazoles, useful as starting material in manufacturing dyes, herbicides, fungicides, etc., were prepared by cyclization of the corresponding 1-benzoyl-3-phenylthioureas with NaNO₂ at 90° followed by hydrolysis at 110-150°. Thus, cyclization of 1-benzoyl-3(2-nitrophenyl)thiourea with NaNO₂ in 96% H₂SO₄ at 50° followed by treatment of the reaction mixture with 20% H₂SO₄ containing H₂NSO₃H and (H₂N)₂CO at 145° afforded 89% 2-amino-4-nitrobenzothiazole.

RX(1) OF 1 A ==> B



RX(1) RCT A 66934-10-9

STAGE(1)

RGT C 7632-00-0 NaNO₂, D 7664-93-9 H₂SO₄

STAGE(2)

RGT D 7664-93-9 H₂SO₄, E 5329-14-6 Sulfamic acid, F
57-13-6 Urea

SOL 7732-18-5 Water

PRO B 6973-51-9

L47 ANSWER 42 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 124:8691 CASREACT

TITLE: 1,2-Diaminobenzimidazoles: selective inhibitors of
nitric oxide synthase derived from aminoguanidine

AUTHOR(S): Hamley, Peter; Tinker, Alan C.

CORPORATE SOURCE: Med. Chem. Dept., R & D Labs., Leicestershire, LE11
ORH, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (1995),
5(15), 1573-6

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

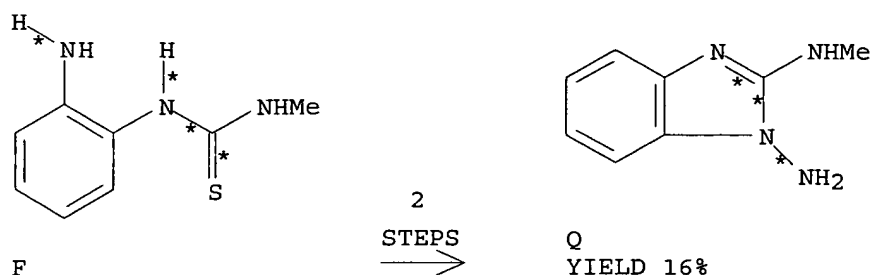
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis of a series of novel 1,2-diaminobenzimidazoles is described. While the parent compound I is a weak, modestly selective inhibitor of the induced isoform of nitric oxide synthase (both mouse and human), a small structural change led to compound II, a highly selective inhibitor of neuronal enzyme.

RX(10) OF 11 COMPOSED OF RX(5), RX(6)

RX(10) F ==> Q



RX (5) RCT F 20367-31-1
 RGT O 74-88-4 Met
 PRO N 17228-38-5
 SOL 64-17-5 EtOH

RX (6) RCT N 17228-38-5
 RGT I 2950-43-8 HOSO₂ONH₂, J 1310-58-3 KOH
 PRO Q 107879-46-9
 SOL 7732-18-5 Water

L47 ANSWER 43 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 122:133069 CASREACT

TITLE: Intramolecular cyclization reaction of amido-ureido (or thioureido)-acetals

AUTHOR(S): Lee, Yong Sup; Kim, Choong Sup; Park, Hokoon

CORPORATE SOURCE: Organic Chem. Lab (I), Korea Inst. Sci. Technology, Seoul, 130-650, S. Korea

SOURCE: Heterocycles (1994), 38(12), 2605-14

CODEN: HTCYAM; ISSN: 0385-5414

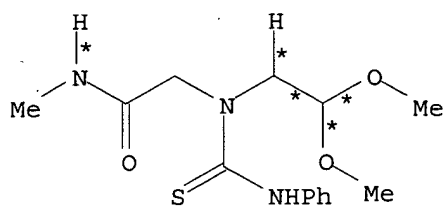
PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

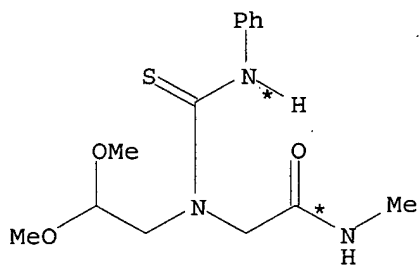
LANGUAGE: English

AB Intramol. cyclization reaction of compds. having amide, urea and acetal functional groups was investigated under various conditions. In acidic conditions, the cyclization reaction of N-methyl-N'-2-(2,2-dimethoxyethyl)-N'-(alkyl- or phenylcarbamoyl)glycine amide proceeded only to afford imidazolinone derivative via an acyliminium ion intermediate formed by intramol. amidoalkylation reaction of amide and acetal functional groups. However, the corresponding compds. having thiourea functional group resulted in the formation of iminothiazolidine derivs. as major product and pyrazinone compds. as minor product. In nearly neutral or basic conditions, both of ureido- or thioureidoacetals afforded hydantoin or thiohydantoin derivs., resp., in excellent yield.

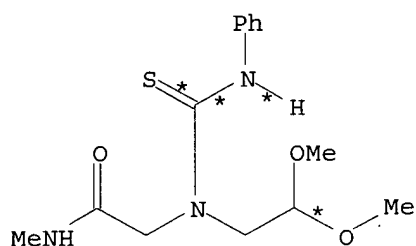
RX (3) OF 33 ...3 F ==> G + H + I



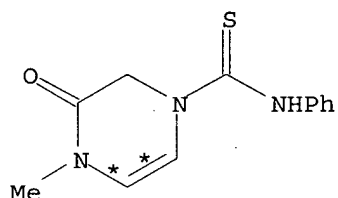
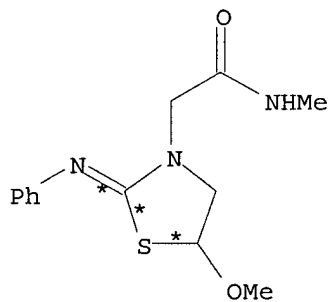
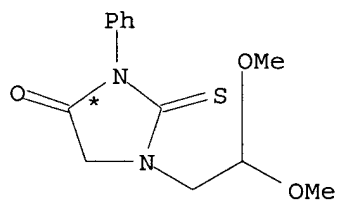
F



F



F

G
YIELD 7%H
YIELD 58%

I

RX(3) RCT F 160952-13-6

STAGE(1)

RGT J 75-75-2 MeSO₃HSOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT K 144-55-8 NaHCO₃

SOL 7732-18-5 Water

PRO G 160952-17-0, H 160952-18-1, I 160952-19-2

NTE REGIOSELECTIVE

L47 ANSWER 44 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 118:254854 CASREACT

TITLE: Synthesis and some reactions of 3-phenyl-(1H,3H)-quinazoline-2-thione-4-one

AUTHOR(S): El-Deen, I. M.; El-Desuky, S.

CORPORATE SOURCE: Fac. Educ., Suez Canal Univ., Egypt

SOURCE: Journal of the Serbian Chemical Society (1992), 57(11), 719-23

CODEN: JSCSEN; ISSN: 0352-5139

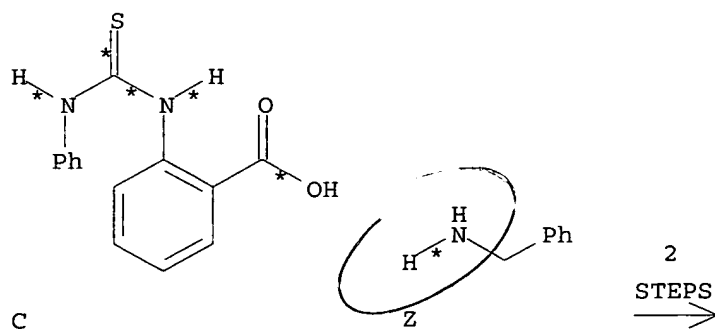
DOCUMENT TYPE: Journal

LANGUAGE: English

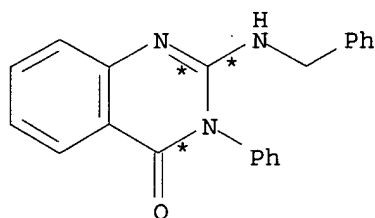
AB Room temperature treatment of 2-(3-Ph thioureido)-benzoic acid with concentrated

sulfuric acid lead to the formation of 3-phenyl(1H,3H)-quinazoline-2-thione-4-one (I) in generally very good yield. Ammonolysis, hydrazinolysis and alkylation of I yielded 2-substituted-3-phenyl(1H,3H)-quinazoline-4-one II (R = NHPh, NHCH₂Ph, NHNH₂, NHNHPh), 3-phenyl-4(1H3H)-quinazolone-2-thioglycolic acid II; R = SCH₂CO₂H) and the ester II (R = SCH₂CO₂Et), resp. Compound II (R = SCH₂CO₂H) reacted with anisaldehyde to afford the β-[3-phenyl-4(1H,3H)-quinazolone-2-yl-thio]-4-methoxystyrene. Treatment of compound II (R = SCH₂CO₂Et) with anthranilic acid gave the corresponding 2-substituted-4H-3,1-benzoxazine-4-one III. Hydrazinolysis and arylation, under Friedel-Crafts conditions, of III affords N-substituted anthranilic acid hydrazide IV (R₁ = NHNH₂) and N-2-(substituted)-benzophenone IV (R₁ = C₆H₃Me₂-2,4), resp.

RX(14) OF 33 COMPOSED OF RX(2), RX(9)

RX(14) C + Z ==> AA

Alternate reaction
yields?



AA

YIELD 75%

RX(2) RCT C 1222-20-4
 RGT F 7664-93-9 H2SO4
 PRO E 18741-24-7

RX(9) RCT E 18741-24-7, Z 100-46-9
 PRO AA 146849-70-9
 SOL 64-17-5 EtOH

L47 ANSWER 45 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 117:48453 CASREACT

TITLE: Polycyclic azines with heteroatoms in the 1- and 3-positions. Part 27. One-pot synthesis of 4-acylimino-2-aminothieno[2,3-d][1,3]thiazines from 2-thioureidothiophene-3-carbonitriles

AUTHOR(S): Guetschow, Michael; Leistner, Siegfried; Pink, Maren
 CORPORATE SOURCE: Sekt. Biowissenschaft., Univ. Leipzig, Leipzig, D-0-7010, Germany

SOURCE: Journal of Heterocyclic Chemistry (1992), 29(2), 279-82

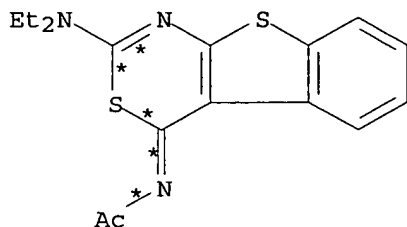
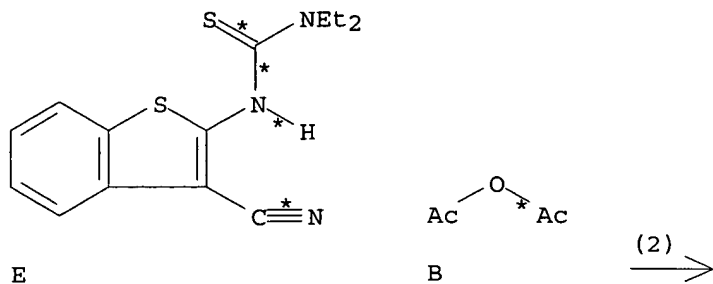
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new one-pot synthesis of 4-acylimino-2-aminothieno[2,3-d][1,3]thiazines I [R1R2 = (CH2)4, R3R4 = (CH2)2O(CH2)2, R5 = Me, Et; R1R2 = (CH2)4, R3 = R4 = Et, R5 = Me, Et; R1 = R2 = Me, R3R4 = (CH2)2O(CH2)2, R5 = Me, Et] from 2-thioureidothiophene-3-carbonitriles II, acetic, propionic anhydride, resp., and concentrated sulfuric acid is reported. The structure of I [R1R2 = (CH2)4, R3R4 = (CH2)2O(CH2)2, R5 = Me] is confirmed by x-ray structure anal.

RX(2) OF 6 E + B ==> F



YIELD 89%

RX(2) RCT E 142310-48-3, B 108-24-7
 RGT D 7664-93-9 H₂SO₄
 PRO F 142310-60-9

L47 ANSWER 46 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 116:151693 CASREACT

TITLE: 2-(3-Acylthioureido)benzonitriles. I. Synthesis and cyclization reactions of 2-(3-acylthioureido)benzonitriles

AUTHOR(S): Pazdera, P.; Potucek, V.; Novacek, E.; Kalvins, I.; Trapencieris, P.; Pugovics, O.

CORPORATE SOURCE: Fac. Nat. Sci., Masaryk Univ., Brno, CS-611 37, Czech.

SOURCE: Chemical Papers (1991), 45(4), 527-40
 CODEN: CHPAEG; ISSN: 0366-6352

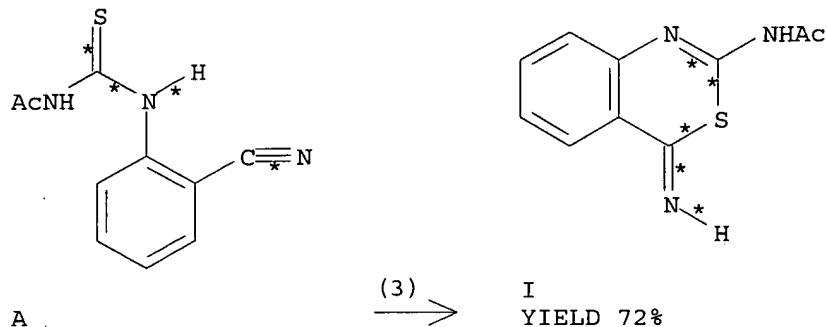
DOCUMENT TYPE: Journal

LANGUAGE: English

AB PhCONHCSNHC6H4COR-o (I; R = OH, NH₂) prepared by the addition of 2-aminobenzonitrile to acylisothiocyanates in acetone solution underwent a cyclization reaction either in concentrated sulfuric acid at room temperature forming acylaminoiminobenzothiazines, e.g., II (R₁ = C₆H₅), or under base catalysis with aqueous solution of sodium hydroxide, ammonia or sodium carbonate at room temperature for II (R₁ = H). This was also prepared by the rearrangement of benzothiazines III (R₂ = Me, OMe, OEt, Ph; X = NH) in aqueous solution of sodium hydroxide. Under the same conditions I (R = OMe) reacted to III (X = O, R₂ = R) and to known 2-thioxo-1,2,3,4-tetrahydroquinazolin-4-one.

This compound is also a product of acid-catalyzed rearrangement of III (X = NH) and III (X = O) rearrangement under acid or base catalysis, resp.

RX(3) OF 8 ...A ==> I...



RX(3) RCT A 119118-96-6
RGT J 7664-93-9 H2SO4
PRO I 138468-37-8

L47 ANSWER 47 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 115:159072 CASREACT

TITLE: Polycyclic azines with heteroatoms in 1- and 3-position. 30. Synthesis of 6,7-dimethoxy substituted 3,1-benzothiazin-4-ones

AUTHOR(S): Guetschow, Michael; Heinecke, Kristina; Thiel, Wilfried; Leistner, Siegfried

CORPORATE SOURCE: Sekt. Biowiss., Univ. Leipzig, Leipzig, O-7010, Germany

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1991), 324(7), 465-6

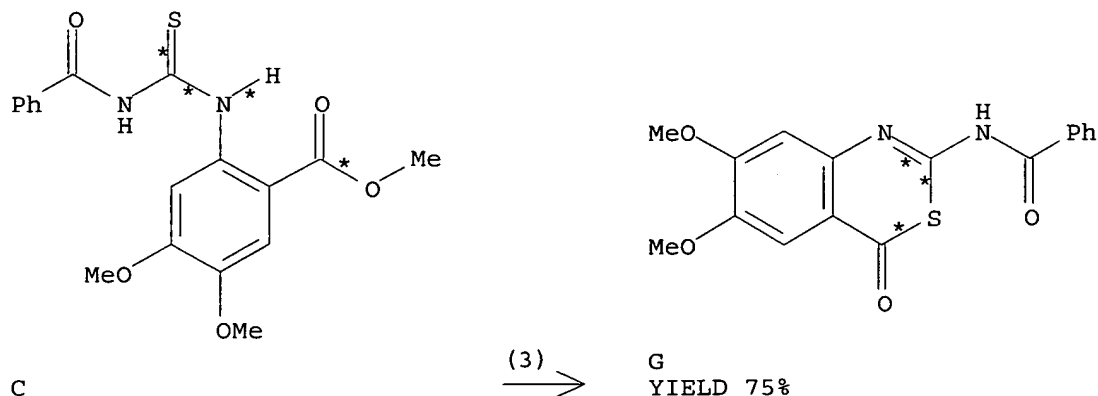
CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Cyclization of the acylthioureas I (R = Me, Ph) gave benzothiazinones II (R = R1 = H; R = Me, R1 = H, Ac, Bz) depending on reaction conditions.

RX(3) OF 10 ...C ==> G



RX(3) RCT C 135509-75-0
 RGT D 7664-93-9 H₂SO₄
 PRO G 135509-76-1

L47 ANSWER 48 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 114:42728 CASREACT

TITLE: Polycyclic azines. XXV. 2-amino-3,1-benzothiazin-4-ones: synthesis, dimroth-rearrangement to quinazolin-4-(3H)-thiones, and MS/MS-fragmentation
 AUTHOR(S): Leistner, Siegfried; Guetschow, Michael; Stach, Joachim

CORPORATE SOURCE: Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1990), 323(10), 857-61

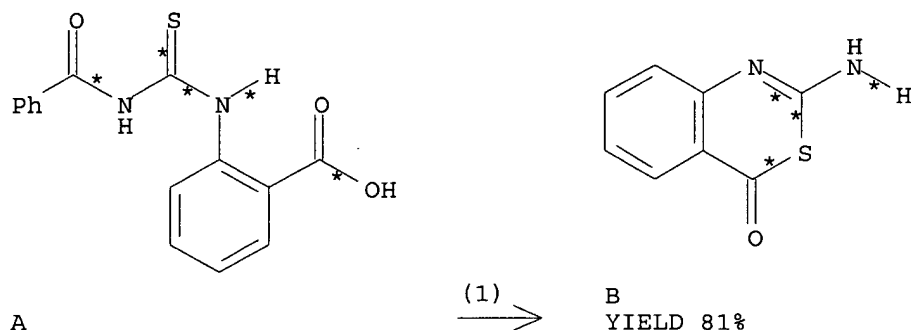
CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German

AB The intramol. cyclocondensation reaction of benzoylthiourea derivs., e.g. 4,2-RR₁C₆H₃NHC(:S)NHCOPh (R = H, Me, Cl; R₁ = CO₂Me, CO₂H, cyano) gave 2-amino-1,3-benzothiazin-4-ones I (same R). Dimroth rearrangement of I gave quinazolin-2-thiones II (same R). The cyclocondensation of 4,2-RR₁C₆H₃NHC(:S)NHCOPh (R = H, Me, Cl; R₁ = CO₂Me, CO₂H) gave 2-(benzoylamino)-1,3-benzothiazin-4-ones. I (R = H) had antianaphylactic activity.

RX(1) OF 9 A ==> B...



RX(1) RCT A 13277-24-2
 RGT C 7664-93-9 H₂SO₄, D 7732-18-5 Water
 PRO B 131357-73-8

L47 ANSWER 49 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 113:6259 CASREACT

TITLE: Multicyclic azines with heteroatoms in the 1- and 3-positions. 24. Preparation of 2-amino-4-iminothieno[2,3-d][1,3]thiazinium salts and their retrocycloaddition reaction to 2-thioureidothiophene-3-carbonitriles

AUTHOR(S): Guetschow, Michael; Leistner, Siegfried

CORPORATE SOURCE: Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.

SOURCE: Zeitschrift fuer Chemie (1990), 30(1), 23-4

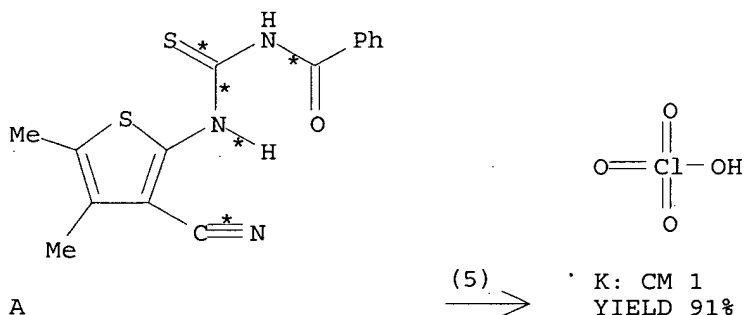
CODEN: ZECEAL; ISSN: 0044-2402

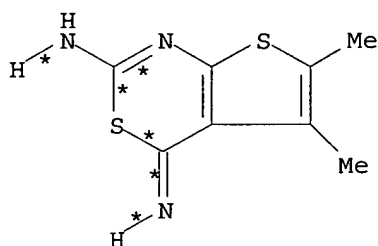
DOCUMENT TYPE: Journal

LANGUAGE: German

AB Treating thiophenecarbonitriles I [R = Me; RR = (CH₂)₄] with H₂SO₄ gave thioureidothiophene-3-carbonitriles, which cyclized to give aminoiminothienothiazinium salts II (X = Cl, ClO₄, HSO₄).

RX(5) OF 11 A ==> K...



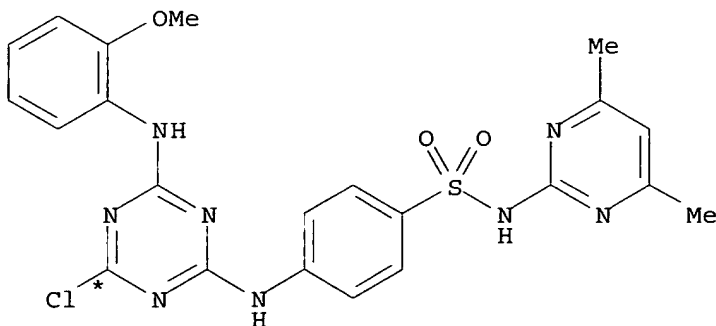


K: CM 2
YIELD 91%

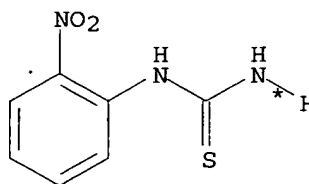
RX(5) RCT A 121746-07-4
RGT C 7664-93-9 H₂SO₄, L 7601-90-3 HClO₄
PRO K 127526-98-1
SOL 7732-18-5 Water

L47 ANSWER 50 OF 82 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 114:164164 CASREACT
TITLE: Synthesis of 2-(2'-methoxyanilino)-4-(2''-p-aminobenzenesulfonamido-4'', 6''-dimethylpyrimidine)-6-(arythioureido)-s-triazine (thiourea derivatives)
AUTHOR(S): Patel, K. H.; Desai, K. R.
CORPORATE SOURCE: Dep. Chem., South Gujarat Univ., Surat, 395 007, India
SOURCE: Proceedings of the National Academy of Sciences, India, Section A: Physical Sciences (1990), 60(1), 7-9
CODEN: PAIAA3; ISSN: 0369-8203
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title compds. I (R = H, o-, m-, p-Me, o-, m-, p-O₂N, o-, m-, p-Cl) were prepared in 3 steps from cyanuric chloride by amination with o-anisidine, amination with sulfadimidine, and amidation with RC₆H₄NHCSNH₂. Maximum inhibition of E. coli occurred with I (R = m-Cl) and for S. aureus with I (R = p-Me).

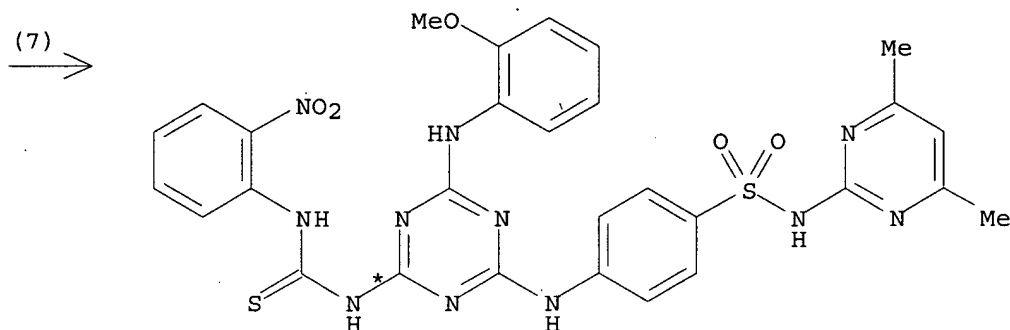
RX(7) OF 42 ... F + O ==> P



F



O



P

RX (7) RCT F 132744-97-9, O 51039-84-0
 PRO P 132744-92-4
 SOL 67-64-1 Me2CO

L47 ANSWER 51 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 112:35587 CASREACT

TITLE: Modified procedure for the preparation of
 5-nitro-2-furylmethylene diacetate and its use in the
 synthesis of some novel (5-nitro-2-furyl)azomethines
 via 5-nitro-2-furaldehyde

AUTHOR(S): Vlaovic, Djordje; Milic, Bozidar L.; Mackenzie,
 Kenneth

CORPORATE SOURCE: Fac. Technol., Univ. Novi Sad, Novi Sad, 21000,
 Yugoslavia

SOURCE: Journal of Chemical Research, Synopses (1989), (6),
 156-7

CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

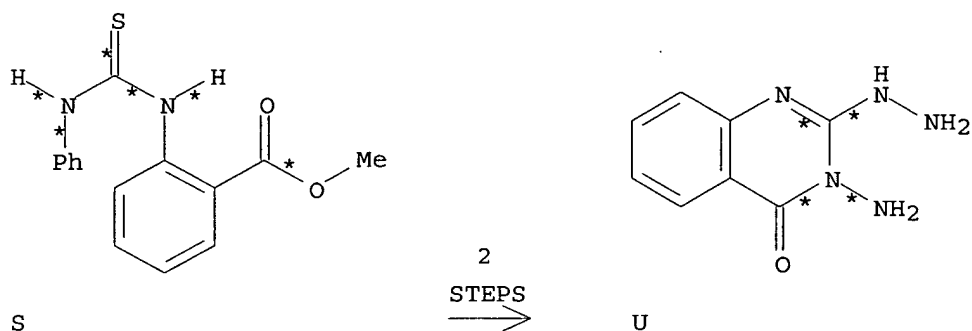
LANGUAGE: English

AB 5-Nitro-2-furylmethylene diacetate (I) was prepared by treating
 2-furaldehyde with Ac2O/fuming HNO3/H2SO4. Acid hydrolysis of I gave
 5-nitro-2-furaldehyde (II). Condensation of II with hydrazines,
 N-amino-substituted N heterocycles, or N-aminoazonium mesitylenesulfonates
 gave the title azomethines. (The sulfonates were prepared by treating N
 heterocycles with 2,4,6-Me3C6H2SO2ONH2). Some examples of the title
 azomethines, e.g., III, were tested as fungicides and bactericides.

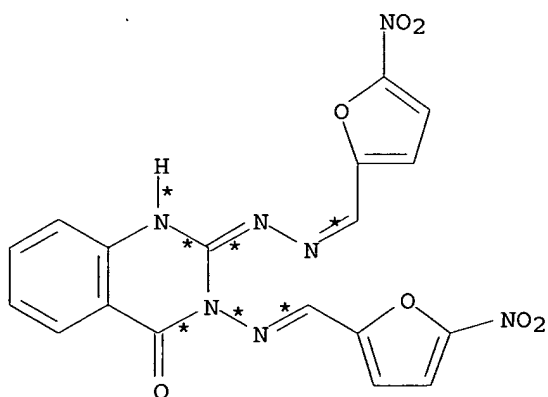
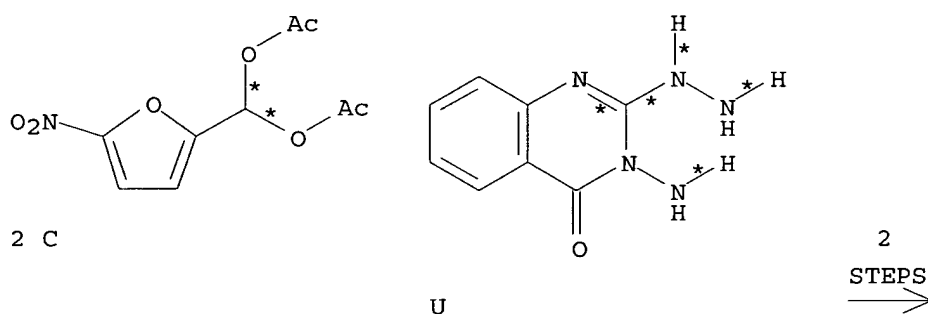
RX(145) OF 191 COMPOSED OF REACTION SEQUENCE RX(7), RX(31)
 AND REACTION SEQUENCE RX(2), RX(31)

... S ==> U...

...2 C + U ==> BU



START NEXT REACTION SEQUENCE



BU
YIELD 100%

RX(7) RCT S 96221-91-9
 RGT J 7803-57-8 N2H4-H2O
 PRO U 19062-39-6

RX(2) RCT C 92-55-7
 RGT G 7732-18-5 Water, E 7664-93-9 H2SO4
 PRO F 698-63-5
 SOL 7732-18-5 Water

RX(31) RCT U 19062-39-6, F 698-63-5
 PRO BU 124608-68-0
 NTE refluxing inert solvent

L47 ANSWER 52 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 110:8117 CASREACT

TITLE: An unambiguous synthesis of 5(6)-substituted
 1-alkoxycarbonylbenzimidazole-2-carbamates

AUTHOR(S): Viswanathan, N.; Sidhaye, A. R.

CORPORATE SOURCE: Pharma Div., Hindustan Ciba-Geigy Ltd. Goregaon,
 Bombay, 400 063, India

SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1988),
 27B(7), 672-3

CODEN: IJSBDB; ISSN: 0376-4699

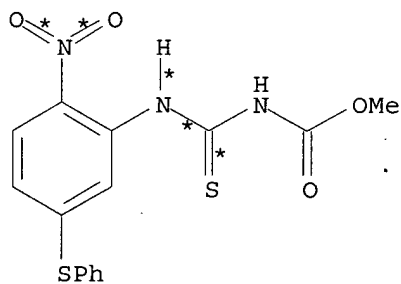
DOCUMENT TYPE: Journal

LANGUAGE: English

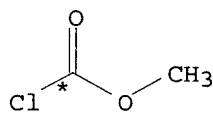
AB Benzothiadiazines I (R1 = SPh, H; R2 = H, OMe) underwent ring contraction
 by treatment with Ph3P to give benzimidazoles II. I were prepared from
 o-nitroanilines by sequential N-thiocarbamoylation, acylation by ClCO2Me,
 reduction-cyclization, and acylation with ClCO2Me.

RX(16) OF 20 COMPOSED OF RX(2), RX(3), RX(4)

RX(16) D + B ==> M

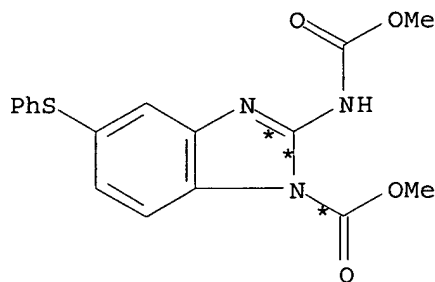


D



B

3
 STEPS
 →



M

RX(2) RCT D 56069-34-2
 RGT G 7775-14-6 Na₂(S₂O₄), H 1310-73-2 NaOH
 PRO F 56068-98-5
 SOL 7732-18-5 Water

RX(3) RCT B 79-22-1, F 56068-98-5
 RGT K 110-86-1 Pyridine
 PRO J 117844-65-2
 SOL 67-66-3 CHCl₃

RX(4) RCT J 117844-65-2
 RGT N 603-35-0 PPh₃
 PRO M 58521-87-2
 SOL 67-66-3 CHCl₃

L47 ANSWER 53 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 109:170390 CASREACT

TITLE: Preparation of 2-[N₄-{N₁-(2'-thiazolyl)sulfanilamido}]-4-(4'-bromoanilino)-6-(substituted-phenylthioureido)-s-triazine and study of their antibacterial activity

AUTHOR(S): Desai, K. R.; Patel, N. B.

CORPORATE SOURCE: Dep. Chem., South Gujarat Univ., Surat, 395 007, India

SOURCE: Journal of the Indian Chemical Society (1988), 65(5), 384-5

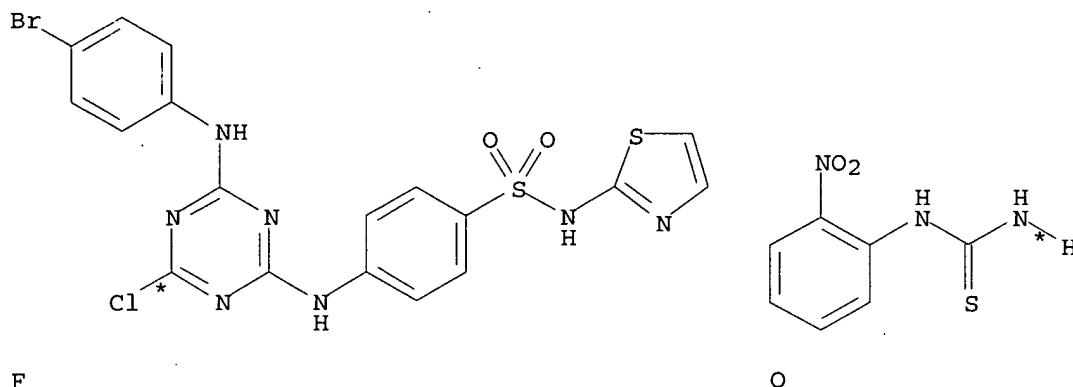
CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

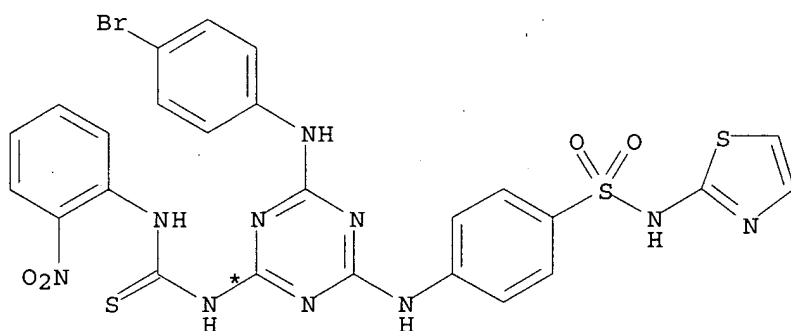
LANGUAGE: English

AB Title compds. I (R = H, o-Me, m-Me, p-Me, o-NO₂, m-NO₂, p-NO₂, o-Cl, p-Cl) were prepared by treating chloro-s-triazine II with the appropriate RC₆H₄NHC(S)NH₂. II was prepared by treating sulfanilamide III with cyanuric chloride and treating the resulting dichloro-s-triazine IV with p-BrC₆H₄NH₂. I exhibited antibacterial activity against Staphylococcus aureus and Escherichia coli.

RX(7) OF 30 ... F + O ==> P



(7) →



RX(7) RCT F 117054-04-3, O 51039-84-0
PRO P 117054-09-8
SOL 67-64-1 Me2CO

L47 ANSWER 54 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 110:75374 CASREACT

TITLE: Condensed derivatives of thiolane 1,1-dioxide. 1.
Synthesis and rearrangement of trans-2-
iminoperhydrothieno[3,4-d]oxazole 5,5-dioxides

AUTHOR(S): Bezmenova, T. E.; Rozhenko, A. B.; Khaskin, G. I.;
Bratunets, A. G.; Shakhvorost, A. M.

CORPORATE SOURCE: Inst. Fiz.-Org. Khim. Uglekhim., Kiev, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1988), (2),
268-71

CODEN: KGSSAQ; ISSN: 0453-8234

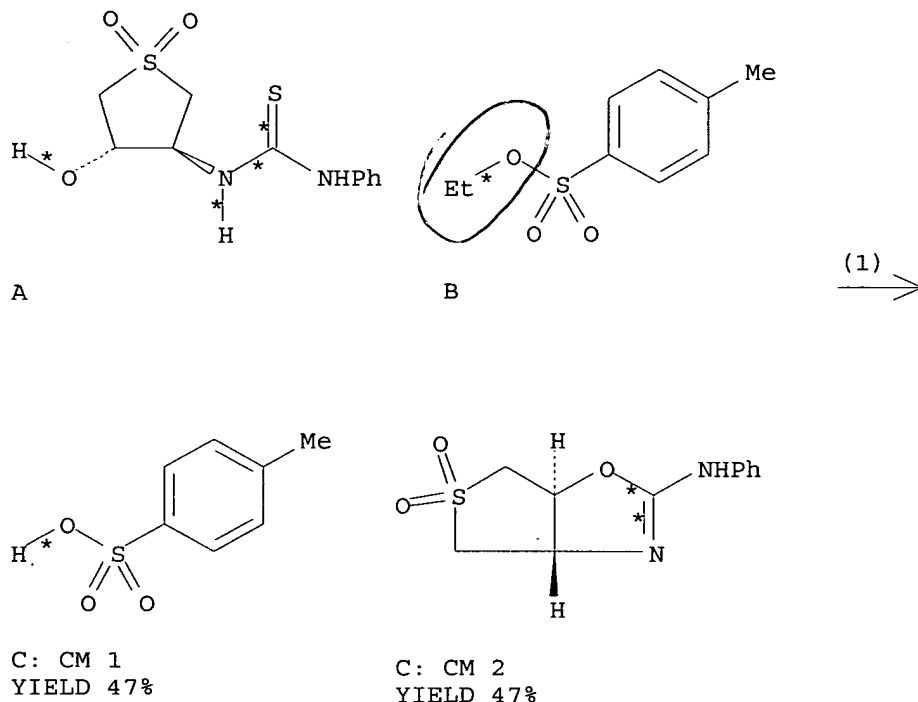
DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Salts of trans-2-iminoperhydrothieno[3,4-d]oxazole 5,5-dioxides I (R = Ph,

PhCH₂, Me₂CH, allyl, Bz) were prepared by alkylating trans-N-alkyl(aryl)-N'-(3-hydroxy-1,1-dioxothiolan-4-yl)thioureas (II) with p-MeC₆H₄SO₃Et, and also by treating trans-3-hydroxy-4-aminothiolane 1,1-dioxides with BrCN. Addnl. obtained were thienoimidazoles III.

RX(1) OF 30 ... A + B ==> C...



RX(1) RCT A 86043-47-2, B 80-40-0
PRO C 118787-42-1

L47 ANSWER 55 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 108:37754 CASREACT

TITLE: The facile synthesis of 2-aminothieno[2,3-d][1,3]thiazin-4-ones, in some cases 5,6-anellated
AUTHOR(S): Leistner, Siegfried; Guetschow, Michael; Wagner, Guenther

CORPORATE SOURCE: Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.

SOURCE: Synthesis (1987), (5), 466-70
CODEN: SYNTBF; ISSN: 0039-7881

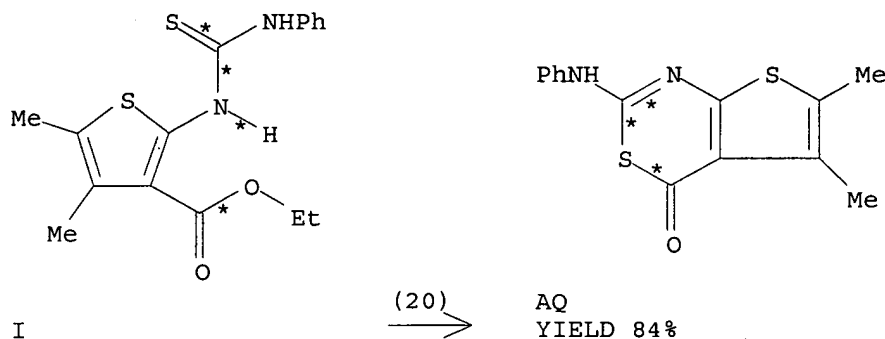
DOCUMENT TYPE: Journal

LANGUAGE: German

AB Acid treatment of Et thioureidothiophenecarboxylates I [R = H, Me; R₁ = Me, Ph; RR₁ = (CH₂)₄, CH₂(NCH₂Ph)(CH₂)₂; R₂ = H, Me, Et; R₃ = H, Me, Me₂CH, cyclohexyl, Ph, Et, 4-HO₂CC₆H₄, 2-pyridyl; R₂R₃ = CH₂CH₂OCH₂CH₂, CH₂CH₂NMeCH₂CH₂, CH₂CH₂N(CH₂CH₂OH)CH₂CH₂, CH₂CH₂N(CH₂CH₂OSO₃H)] with H₂SO₄, HClO₄, or polyphosphoric acid gave aminothienothiazinones II (X = O). Thiolation of II (R = R₁ = Me, R₂ = H, R₃ = Ph, X = O; R = R₁ = Me,

R2R3 = CH₂CH₂OCH₂CH₂, X = O) with P2S5 gave II (X = S). Ring cleavage reactions of II with NaOH gave thioureidothiophenecarboxylic acids III (R₂,R₃ = Me; R₂R₃ = CH₂CH₂OCH₂CH₂, CH₂CH₂NMeCH₂CH₂).

RX(20) OF 74 ...I ==> AQ...



RX(20) RCT I 59898-45-2
RGT AR 7664-93-9 H₂SO₄
PRO AQ 105544-46-5

L47 ANSWER 56 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 108:94454 CASREACT

TITLE: Synthesis of thiazole derivatives with positive inotropic effect

AUTHOR(S): Kosary, Judit; Kasztreiner, E.; Rabloczky, G.; Vitalis, Beata

CORPORATE SOURCE: Inst. Drug Res., Budapest, H-1325, Hung.

SOURCE: Pharmazie (1987), 42(6), 373-5

CODEN: PHARAT; ISSN: 0031-7144

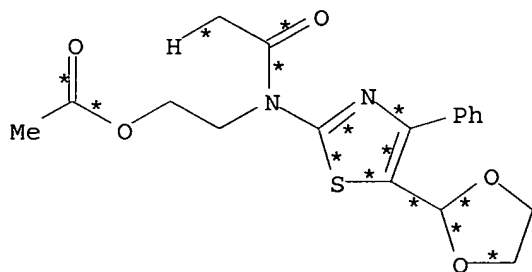
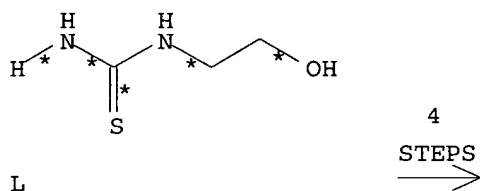
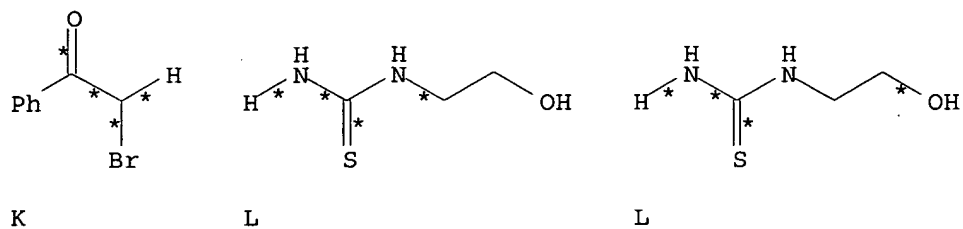
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Thiazole I (R = H) was prepared by cyclocondensation of PhCOCHBrCO₂Et with HOCH₂CH₂NHCSNH₂. I (R = Ac) was prepared by acetylation of I (R = H). Thioxooxazolidinylthiazole II was prepared by cyclization of I (R = H) with CSCL₂. I (R = Ac) and II have medium pos. inotropic effects equal to that of isoprotenerol at 5 mg/kg in the cat. Other thiazole derivs. were prepared but possessed weak inotropic activities.

RX(72) OF 86 COMPOSED OF RX(7), RX(26), RX(27), RX(29)

RX(72) K + 3 L ==> BK



BK
YIELD 53%

RX(7) RCT K 70-11-1, L 29146-81-4
 RGT N 127-09-3 AcONa
 PRO M 77627-63-5
 SOL 64-17-5 EtOH

RX(26) RCT M 77627-63-5
 RGT AB 108-24-7 Ac2O
 PRO BE 113019-82-2
 CAT 7664-93-9 H2SO4

RX(27) RCT BE 113019-82-2
 RGT BG 10025-87-3 POCl3
 PRO BF 113019-83-3
 SOL 68-12-2 DMF

RX(29) RCT BF 113019-83-3
 RGT AX 107-21-1 (CH2OH)2, BL 98-59-9 TsCl
 PRO BK 113019-85-5
 SOL 71-43-2 Benzene

L47 ANSWER 57 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 105:133804 CASREACT

TITLE: New 2-aryliminoimidazolidines. I. Synthesis and antihypertensive properties of 2-(2-phenoxyphenylimino)imidazolidines and related compounds

AUTHOR(S): Matsuo, Masaaki; Taniguchi, Kiyoshi; Katsura, Yousuke; Kamitani, Toshiharu; Ueda, Ikuo

CORPORATE SOURCE: Cent. Res. Lab., Fujisawa Pharm. Co., Ltd., Osaka, 532, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(10), 4409-21

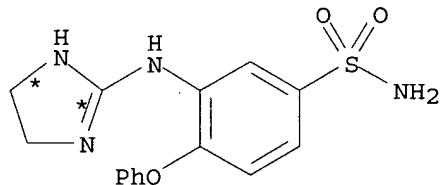
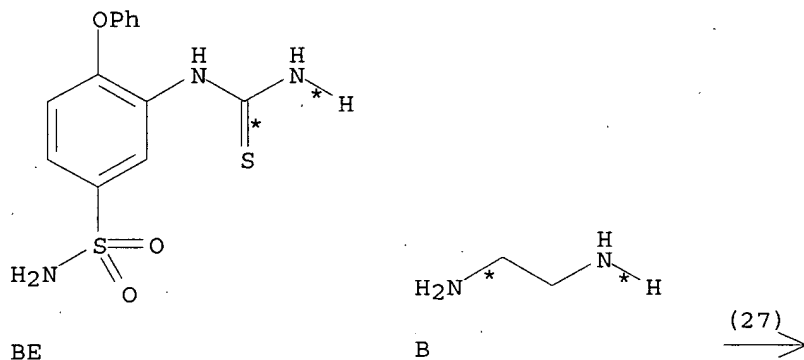
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 2-(2-Phenoxyphenylimino)imidazolidines I (R = Ph, substituted Ph, R1 = H; R = Ph, R1 = Cl, Me, NO2, cyano, amino, SO2NH2, CF3, OH, OMe, SO2NMe2; R = 4-ClC6H4, R1 = 5-Cl, 5-Me) and related compds. were synthesized and evaluated for hypotensive activity in rats. Most I were synthesized via the aniline derivs. by two different methods. Some were significantly hypotensive, with I (R = Ph, R1 = 5-Cl) may involve the blockade of peripheral α -adrenergic receptors.

RX(27) OF 382 ...BE + B ==> BF



RX(27) RCT BE 76839-36-6

STAGE(1)

RGT D 74-88-4 MeI

SOL 67-56-1 MeOH

STAGE(2)

RCT B 107-15-3

SOL 64-17-5 EtOH

PRO BF 76841-37-7

L47 ANSWER 58 OF 82 CASREACT. COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 103:196032 CASREACT

TITLE: New antihistaminic N-heterocyclic 4-piperidinamines.

3. Synthesis and antihistaminic activity of

N-(4-piperidinyl)-3H-imidazo[4,5-b]pyridin-2-amines

AUTHOR(S): Janssens, Frans; Torremans, Joseph; Janssen, Marcel;
Stokbroekx, Raymond A.; Luyckx, Marcel; Janssen, Paul
A. J.

CORPORATE SOURCE: Res. Lab., N. V. Janssen Pharm., Beerse, B-2340, Belg.

SOURCE: Journal of Medicinal Chemistry (1985), 28(12), 1943-7

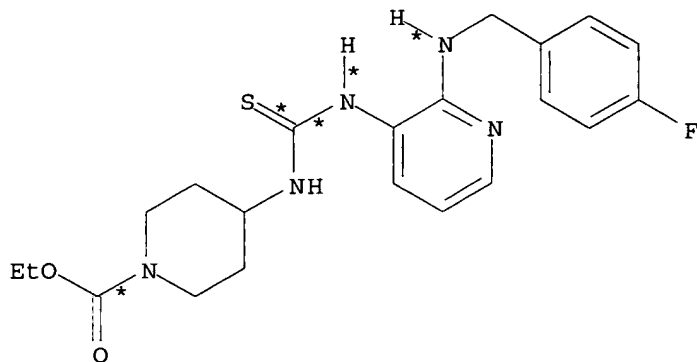
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

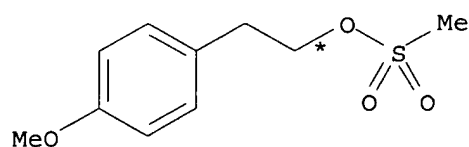
LANGUAGE: English

AB To study the bioisosteric replacement of a 2-pyridyl ring for a Ph nucleus in astemizole, a series of N-(4-piperidinyl)-3H-imidazo[4,5-b]pyridin-2-amines I [R = H, F; R1 = (un)substituted alkyl] was synthesized and evaluated. The title compds. were obtained starting from either I (R1 = H) by 4 synthetic methods. The in vivo antihistamine activity was evaluated by the compound 48/80-induced lethality test in rats and the histamine-induced lethality test in guinea pigs after oral and/or s.c. administration. Compound I (R = F, R1 = p-MeOC6H4CH2CH2), the isostere of astemizole, showed the most potent antihistaminic properties in the rat. However, astemizole is superior to I (R = F, R1 = p-MeOC6H4CH2CH2) as to duration of action and total potency.

RX(39) OF 52 COMPOSED OF RX(8), RX(10), RX(11)

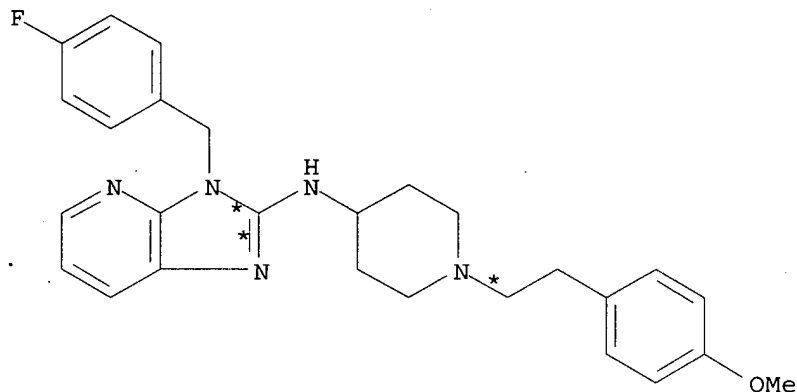
RX(39) O + Y ==> Z

O



Y

3
STEPS
→



Z

RX(8) RCT O 75971-36-7
 RGT Q 21908-53-2 HgO
 PRO T 73733-99-0
 CAT 7704-34-9 S
 SOL 109-99-9 THF

RX(10) RCT T 73733-99-0
 RGT V 10035-10-6 HBr
 PRO X 75979-00-9
 SOL 7732-18-5 Water

RX(11) RCT Y 73735-36-1, X 75979-00-9
 RGT D 497-19-8 Na2CO3
 PRO Z 73755-88-1
 SOL 68-12-2 DMF

L47 ANSWER 59 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 104:168731 CASREACT

TITLE: Nucleoside complexing. A carbon-13 NMR spectroscopic investigation of the metal binding sites in 7-methylguanosine, 7-methylinosine and some related new synthetic betaines

AUTHOR(S): Shinozuka, Kazuo; Wilkowski, Kenneth; Heyl, Barbara L.; Marzilli, Luigi G.

CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA

SOURCE: Inorganica Chimica Acta (1985), 100(1), 141-50

CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE:

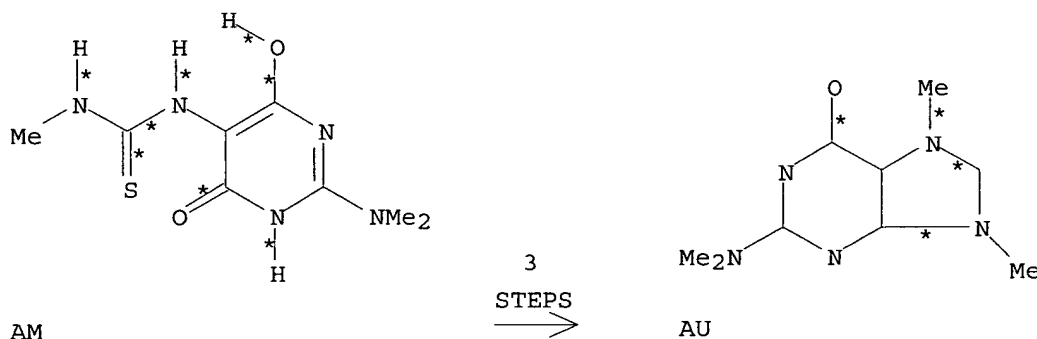
Journal

LANGUAGE:

English

AB A ¹³C NMR spectroscopic study of the binding of various metal species, including hard metal species (Sr, Ba, La, Pr), intermediate metal species (Zn, Cd, Pb), and soft metal species (Pt, Hg), is reported. The ¹³C NMR shift patterns for the O6 resonance of 7-methylguanosine, 7-methylinosine, 2-(dimethylamino)-7.9-dimethylhypoxanthinium betaine, 2-(diethylamino)-7-methyl-9-propylhypoxanthinium betaine, and the (ethylamino) and 6-thio analogs of the latter betaine suggest that metal species of intermediate 'softness' prefer endocyclic N1 binding over exocyclic O6 to a larger extent than they prefer endocyclic N3 binding over exocyclic O2 binding in cytosine derivs. 2-Dimethylamino-9-methylhypoxanthine I (R,R1 = Me; R2 = Me) was prepared from 5-amino-4,6-dihydroxy-2-dimethylaminopyrimidine II (R3 = NH₂, R4 = OH, R5 = NMe₂) by addition of MeNCS, ring closure with HCL, and Raney nickel desulfurization. I (R,R1 = H, Et; R2 = Pr) were prepared from II (R3 = NO₂, R4 = NH₂, R5 = SMe) by treatment with Me₂NH, EtNH₂, or Et₂NH followed by cycloaddns. with Na₂S₂O₄, HCO₂H₂ and CHCONH₂ alkylation with alkyl halides, and deamination with HNO₂. I were methylated to give the corresponding hypoxanthinium betaines III.

RX(70) OF 89 COMPOSED OF RX(20), RX(21), RX(23)

RX(70) AM ==> AU

RX(20) RCT AM 101479-46-3
 RGT AO 7647-01-0 HCL
 PRO AN 101504-39-6

RX(21) RCT AN 101504-39-6
 RGT AQ 7440-02-0 Ni, J 1310-73-2 NaOH
 PRO AP 36323-96-3
 SOL 7732-18-5 Water
 NTE Raney nickel

RX(23) RCT AP 36323-96-3
 RGT U 77-78-1 Me₂SO₄
 PRO AU 101479-47-4
 SOL 127-19-5 AcNMe₂

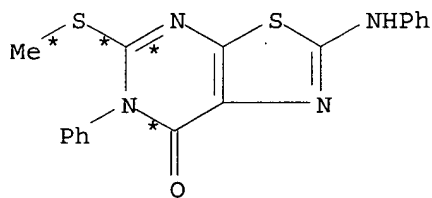
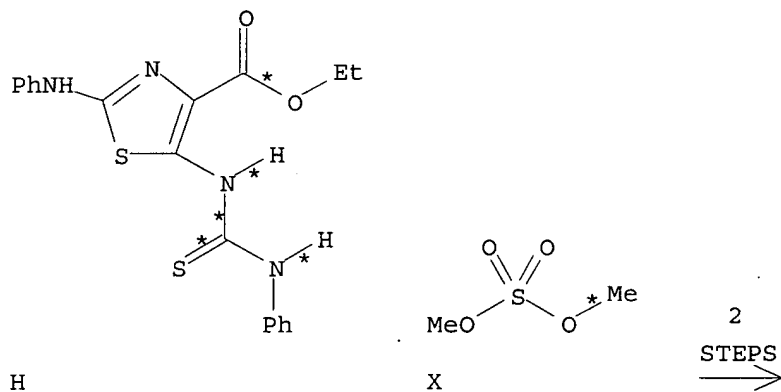
L47 ANSWER 60 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 99:122400 CASREACT
 TITLE: Studies on fused-ring mesoionic thiazolo[3,2-a]thiazolo[5,4-d]pyrimidine system
 AUTHOR(S): Talukdar, P. B.; Sengupta, S. K.; Datta, A. K.
 CORPORATE SOURCE: Res. Dev. Div., East India Pharm. Works Ltd., Calcutta, 700 061, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(3), 243-8
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Cyclodehydration of 5-carboxymethylmercaptothiazolo[5,4-d]pyrimidine-7(6H)-ones I (R = SMe, NHPh; R1 = Me, Ph; R2 = Ph) with Ac2O readily affords new fused-ring mesoionic systems II. I (R2 = H) fail to give pure products under similar treatment, but the thiazolium perchlorate, III were acylated to give pure mesoionic ketones II (R = SMe, R1 = Me, R2 = Ac, COC6H4NO2-4). II furnish alc. adducts.

RX(28) OF 36 COMPOSED OF RX(8), RX(16)

RX(28) $\underline{H} + \underline{X} \implies \underline{Y}$



RX(8) RCT H 86998-84-7
 PRO L 86998-88-1

RX(16) RCT L 86998-88-1, X 77-78-1

PRO Y 86998-89-2

L47 ANSWER 61 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 99:38400 CASREACT

TITLE: Secondary products of sulfonamides. 5.
2-(Arenesulfonylimino) Δ 4-thiazolines from
2-(arenesulfonylimino)-1,3-oxathioles

AUTHOR(S): Hans, Martin; Dehne, Heinz

CORPORATE SOURCE: Sekt. Biol./Chem., Paedagog. Hochsch. "Liselotte
Herrmann", Guestrow, DDR-2600, Ger. Dem. Rep.

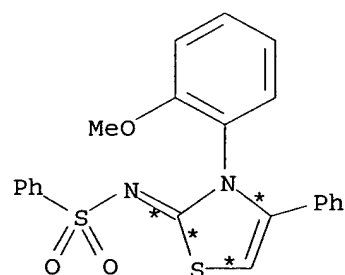
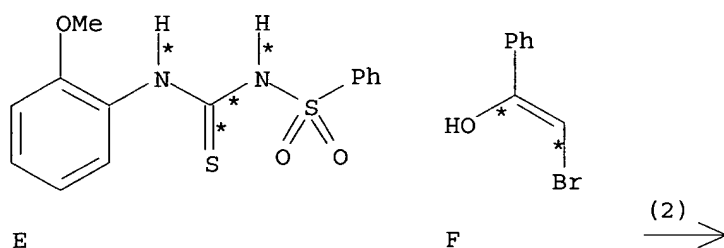
SOURCE: Zeitschrift fuer Chemie (1983), 23(2), 54

CODEN: ZECEAL; ISSN: 0044-2402

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Iminothiazoles I (X = NC₆H₄R₂; R = H, Me, Cl; R₁ = H, NO₂; R₂ = H, 2-MeO, 4-MeO, 4-Cl) were obtained in 51-87% yield by treating I (X = O) with R₂C₆H₄NH₂ and HOAc. I (X = 2-MeOC₆H₄N, R = R₁ = H) was obtained by treating PhSO₂N:C(SH)NHC₆H₄OMe-2 with BrCH₂Bz. I (X = NC₆H₄R₂, R = H, R₁ = NO₂, R₂ = H, 2-MeO) were also prepared by this method.

RX(2) OF 10 E + F ==> G

G

RX(2) RCT E 70318-85-3, F 344397-97-3PRO G 86379-74-0

SOL 67-56-1 MeOH

L47 ANSWER 62 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 64:36155 CASREACT

TITLE: Synthetic nucleosides. LXVI. Studies on the synthesis of cis-2,3-diamino sugars. 6. Neighboring group reactions with methyl 4,6-O-benzylidene-3-deoxy-2-O-methylsulfonyl-3-thioureido- α -D)-glucopyranoside

AUTHOR(S): Baker, B. R.; Hullar, T. L.

CORPORATE SOURCE: State Univ. of New York, Buffalo

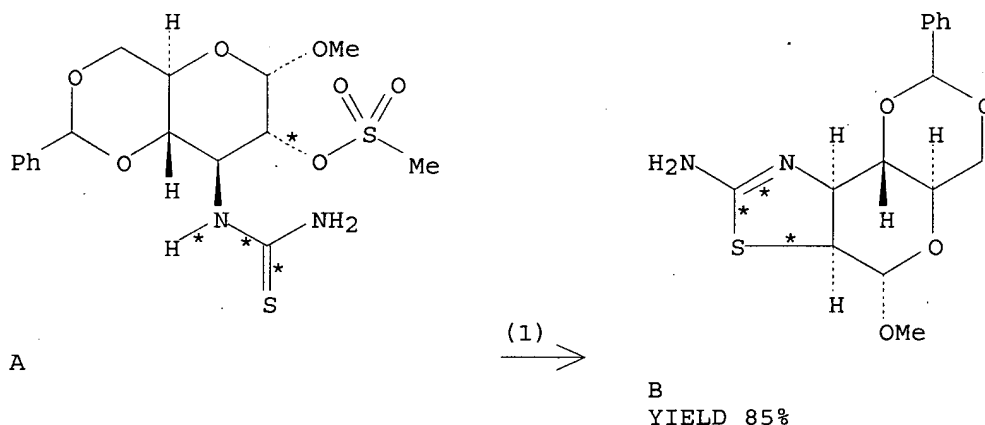
SOURCE: Journal of Organic Chemistry (1965), 30(12), 4045-8
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB cf. preceding abstract Methyl 4,6-O-benzylidene-3-deoxy-2-O-methylsulfonyl-3-thioureido- α -D-glucopyranoside (I) was cyclized in pyridine or in methanolic sodium methoxide solution to give the thiazoline, 2-amino-4',6'-O-benzylidene-1'-O-methyl- α -D-mannopyrano [3',2':4,5] - 2 - thiazoline (II). These results further confirm the view that in a strongly basic medium a sugar derivative possessing a nucleophilic trifunctional neighboring group and a suitable leaving group in a trans-diequatorial disposition will cyclize to form a five-membered ring rather than the thermodynamically less stable aziridine.

RX(1) OF 1 A ==> B



RX(1) RCT A 5983-26-6
RGT C 75-75-2 MeSO₃H
PRO B 6038-66-0
SOL 110-86-1 Pyridine, 141-78-6 AcOEt
NTE Classification: Cyclisation; Heterocycle formation;
Condensation; # Conditions: pyridine Rf 2h; MsOH EtOAc; #
Comments: product as MsOH salt

L47 ANSWER 63 OF 82 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 64:36154 CASREACT

TITLE: Synthetic nucleosides. LXV. Studies on the synthesis of cis-2,3-diamino sugars. 5. Neighboring group reactions with derivatives of methyl 2-amino-4,6-O-benzylidene-2-deoxy- α -D-altropyranoside

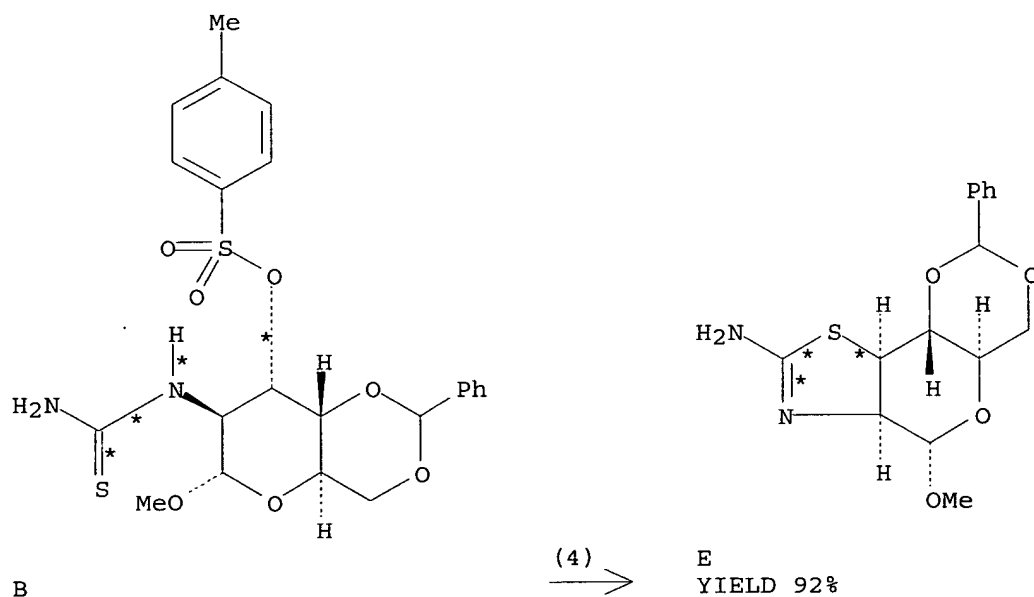
AUTHOR(S): Baker, B. R.; Hullar, T. L.

CORPORATE SOURCE: State Univ. of New York, Buffalo
 SOURCE: Journal of Organic Chemistry (1965), 30(12), 4038-44
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB cf. CA 60, 15954f; 63, 5717b. Treatment of methyl 4,6-O-benzylidene-N-cyano-2-deoxy-2-(p-toluenesulfonamido)-3-O-(p-tolylsulfonyl)- α -D-altropyranoside (I) with hydrogen sulfide gave the N-detosylated thioureido derivative, methyl 4,6-O-, benzylidene-2-deoxy-3-O-(p-tolylsulfonyl)-2-thioureido- α -D-altropyranoside (II). Cyclization of II in pyridine or ethanolic solution gave 2-amino-4',6'-O-benzylidene-1'-O-methyl- α -D-mannopyrano[2',3':4,5]-2-thiazoline (III). In contrast, anionic cyclization of the ureido derivative, methyl 4,6-O-benzylidene-2-deoxy-3-O-(p-tolylsulfonyl)-2-ureido- α -D-altropyranoside (IV), gave the aziridine, methyl 4,6-O-benzylidene-N-carbamoyl-2,3-dideoxy-2,3-imino- α -D-mannopyranoside (V). These results further confirm the generality that formation of aziridines readily occurs when the requisite substituents are trans-diaxial to each other. Addition of benzylamine to 10a gave, after cyclization and hydrolysis, a derivative of 2,3-diamino-2,3-dideoxy-D-mannose.

RX(4) OF 5 ...B ==> E



RX(4) RCT B 6167-99-3
 PRO E 6038-63-7
 SOL 64-17-5 EtOH
 NTE Classification: Heterocycle formation; Cyclisation;
 Isomerisation; Condensation; # Conditions: EtOH Rf 30mn; #
 Comments: product as TsOH salt

L47 ANSWER 64 OF 82 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 60:91148 CASREACT

TITLE: Synthetic nucleosides. LIX. Studies on the synthesis of cis-2,3-diamino sugars. 2. The thiourea neighboring group

AUTHOR(S): Baker, B. R.; Neilson, Thomas

CORPORATE SOURCE: State Univ. of New York, Buffalo

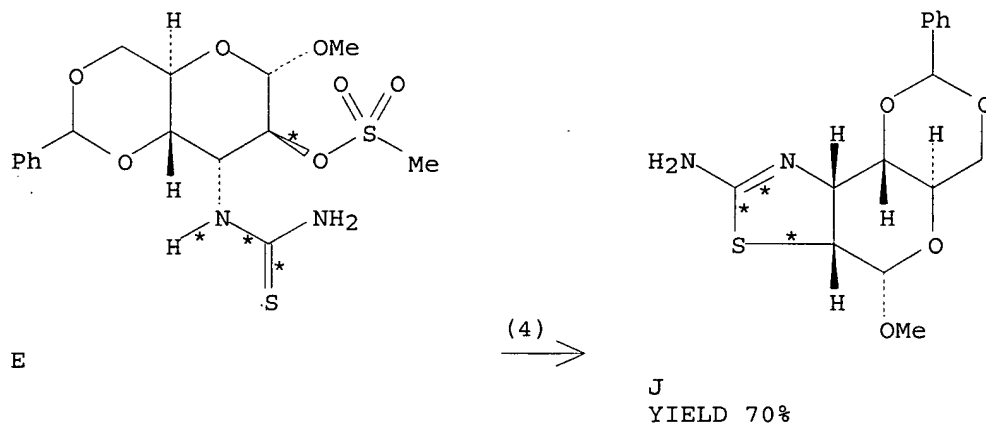
SOURCE: Journal of Organic Chemistry (1964), 29(5), 1051-6
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Neighboring group ring closure of the N-thiocarbamoyl derivative (I) of Me 3-amino-4,6-O-benzylidene-3-deoxy-2-O-mesyl- α -D-altropyranoside under acid acceptor conditions gave a thiazolino sugar (II). When the anion of I was cyclized, an N-thiocarbamoylimine derivative (III) was obtained rather than the expected imidazoline. That the ring closure of I to III could not be attributed to the fixed trans-diaxial conformations of attacking and leaving groups was shown by the anionic ring closure of IV. (MS = mesyl); since the participating groups in the anionic ring closure of IV can assume either trans-diaxial or trans-diequatorial conformations with little energy difference, the formation of the N-thiocarbamoyl imine rather than an imidazoline must be attributed to factors apparently more important than the conformational factors. The N-thiocarbamoyl derivative (V) of Me 2-amino-4,6-O-benzylidene-2-deoxy-3-O-mesyl- β -D-glucopyranoside, which has trans-diequatorial participating groups, ring-closed to a thiazoline (VI) under acid acceptor conditions. In contrast to I, anionic ring closure of V did not lead to N attack to form either an imine or an imidazoline; S attack took place to give the same thiazoline (VI) obtained under acid acceptor conditions.

RX(4) OF 4 E ==> J



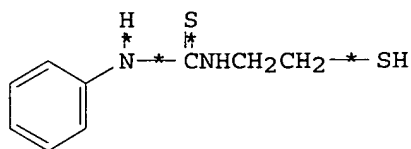
RX(4) RCT E 106759-07-3
PRO J 557099-35-1
SOL 110-86-1 Pyridine
NTE Classification: Cyclisation; Heterocycle formation;
Condensation; Diastereoselective; # Conditions: pyridine Rf 1h

=> d bib ab fhit 65

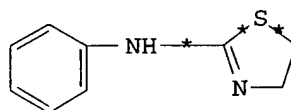
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' - CONTINUE?
(Y)/N:y

✓
 L47 ANSWER 65 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN
 AN 200506046 CHEMINFORMRX
 TI A Convenient Method for the Synthesis of 2-Amino Substituted
 aza-Heterocycles from N,N'-Disubstituted Thioureas Using TsCl/NaOH.
 AU HEINELT, U.; SCHULTHEIS, D.; JAEGER, S.; LINDENMAIER, M.; POLLEX, A.;
 BECKMANN, H. S. G.
 CS Aventis Pharma Dtschl. GmbH, D-65926 Frankfurt/M., Germany
 SO Tetrahedron, 60(44), 9883-9888 (2004)
 CODEN: TETRAB ISSN: 0040-4020
 LA English

RX(5) OF 13 O ==> P



VI



VII
 YIELD 32.0%

RX(5) RCT VI, 1059911
 RGT 1179 (98-59-9), TosCl
 1159 (1310-73-2), NaOH
 SOL 206 (109-99-9), THF
 222 (7732-18-5), H2O
 PRO VII, 887254
 YDS 32.0 %
 KW alkylation; S-alkylation
 NTE reaction:VI -> VII

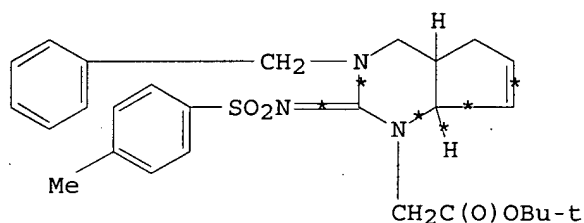
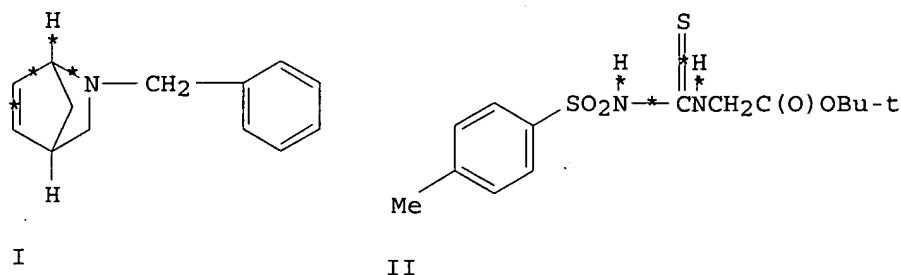
=> d bib ab fhit 66-82

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' - CONTINUE?

(Y)/N:y

✓
 L47 ANSWER 66 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN /
 AN 200502157 CHEMINFORMRX
 TI A 1,3-Diaza-Claisen Rearrangement that Affords Guanidines.
 AU BOWSER, A. M.; MADALENGOITIA, J. S.
 CS Dep. Chem., Univ. Vt., Burlington, VT 05405, USA
 SO Org. Lett., 6(19), 3409-3412 (2004)
 CODEN: ORLEF7 ISSN: 1523-7060
 LA English
 AB The first example of a zwitterionic 1,3-diaza-Claisen rearrangement to
 give guanidine products is presented. The reaction proceeds in modest to
 good yields and is fairly functional group tolerant.

RX(3) OF 8 A + H ==> I



YIELD 71.0%

RX(3) RCT I, 481150
 II, 1056632
 RGT 1087 (1892-57-5), EDC
 SOL 60 (75-09-2), CH₂Cl₂
 PRO III, 1056633
 YDS 71.0 %
 T 25.0 Cel
 TIM 16 hr
 KW alkylation; N-alkylation
 NTE reaction: I (II) -> III, example: 3

~~L47 ANSWER 67 OF 82 CHEMINFORMRX COPYRIGHT 2007-FIZ-CHEMIE on-STN~~

AN 200418091 CHEMINFORMRX

TI Synthesis and Transformations of 3-Ethoxycarbonyl-2-(N-R-thioureido)thiophenes.

AU CHUMAKOVA, L. Y.; DEMCHENKO, A. M.; KRASOVSKY, A. N.; DOLISHNYAK, T. V.; LOZINSKII, M. O.

CS Shevchenko Pedagog. Univ., Chernigov 250037, Ukraine

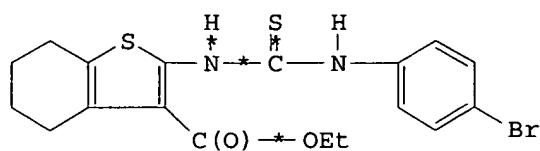
SO Chem. Heterocycl. Compd. (N. Y.), 39(8), 1002-1012 (2003)

CODEN: CHCCAL ISSN: 0009-3122

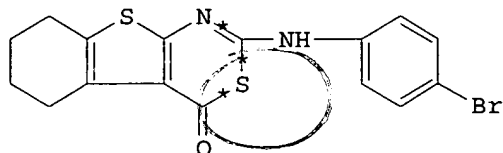
LA English

AB The synthesis of title thioureido-tetrahydrobenzothiophenes (III) is smoothly achieved by reaction of the corresponding isothiocyanate (I) with primary or secondary amines (II). Cyclization proceeds in the presence of acid to furnish thiazino-fused tetrahydrobenzothiophenes like (V), while the pyrimidino-fused analogues (IV) and (VIII) are obtained under alkaline conditions. Further alkylation proceeds at the sulfur exclusively [cf. (X)].

RX(14) OF 34 ...H ==> AA



III

(14)
→

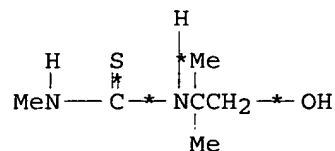
V

YIELD 67.0%

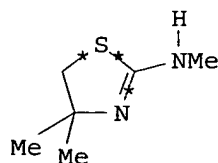
RX(14) RCT III, 1005144
 RGT 198 (7664-93-9), H₂SO₄
 PRO V, 1005155
 YDS 67.0 %
 T 18.0 - 20.0 Cel
 KW acylation; S-acylation
 NTE reaction: IIIc -> V

✓ I47 ANSWER 68 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN
 AN 200326075 CHEMINFORMRX
 TI N-Benzyloxycarbonyl-2-methylaminothiazoline as a Selective
 Benzyloxycarbonylating Reagent of Amines.
 AU KIM, T. H.; CHUN, J. C.
 CS Fac. Appl. Chem., Chonnam Natl. Univ., Kwangju 500-757, S. Korea
 SO Bull. Korean Chem. Soc., 24(2), 157-158 (2003)
 CODEN: BKCSDE ISSN: 0253-2964
 LA English
 AB N-Benzyloxy- and N-t-butoxycarbonyl-2-methylaminothiazolines (VI) serve as
 new agents for the selective alkoxy carbonylation of less hindered amines
 in the presence of more hindered amines.

RX(2) OF 36 ...C ==> E...



III

(2)
→

IV

YIELD 83.0%

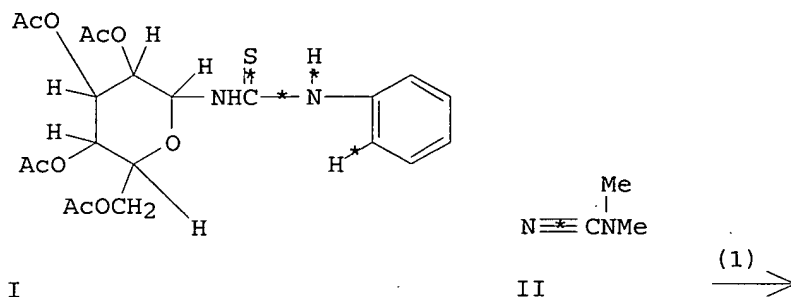
RX(2) RCT III, 683225
 RGT 1179 (98-59-9), TosCl

1159 (1310-73-2), NaOH
 SOL 206 (109-99-9), THF
 PRO IV, 932241
 YDS 83.0 %
 T 25.0 Cel
 KW alkylation; S-alkylation
 NTE reaction:III -> IV

L47 ANSWER 69 OF 82-CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 200317174 CHEMINFORMRX
 TI Novel and Efficient Synthesis of 4-Dimethylamino-2-glycosylaminoquinazolines by Cyclodesulfurization of Glycosyl Thioureas with Dimethylcyanamide.
 AU GAMA, Y.; SHIBUYA, I.; SHIMIZU, M.
 CS Natl. Inst. Adv. Ind. Sci. Technol., Tsukuba, Ibaraki 305, Japan
 SO Chem. Pharm. Bull., 50(11), 1517-1519 (2002)
 CODEN: CPBTAL ISSN: 0009-2363
 LA English
 AB Mechanistical aspects are discussed.

RX(1) OF 4 A + B ==> C



III
 YIELD 67.0%

RX(1) RCT I, 940681, CHIRAL
 II, 9255 (1467-79-4)
 STAGE(1)
 RGT 695 (2923-28-6), AgOTf
 T 100.0 Cel
 STAGE(2)
 RGT 1159 (1310-73-2), NaOH
 SOL 83 (141-78-6), Et-O-Ac
 PRO III, 940682, CHIRAL

YDS 67.0 %

KW aromatisation; alkylation; N-alkylation; C-alkylation; arylation

NTE reaction: I* 1.(II) -> III*, example: 1

L47 ANSWER 70 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 200228057 CHEMINFORMRX

TI Investigation of the Cyclization of N-(2-Hydroxyethyl)-N'-phenylthioureas: Mitsunobu Conditions vs TsCl/NaOH System.

AU LEE, G.-J.; KIM, J. N.; KIM, T. H.

CS Fac. Appl. Chem., Chonnam Natl. Univ., Kwangju 500-757, S. Korea

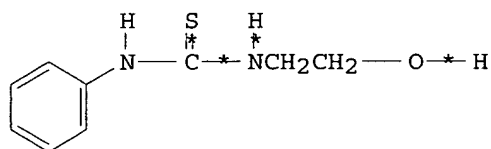
SO Bull. Korean Chem. Soc., 23(1), 19-20 (2002)

CODEN: BKCSDE ISSN: 0253-2964

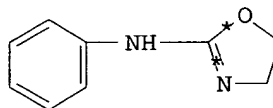
LA English

AB Intramolecular Mitsunobu reaction of the title N-hydroxyethylthioureas (I) provides mainly N- and S-cyclization products (II) and (III), resp., while regioselective formation of O-alkylation products (IV) is observed in TosCl/NaOH-mediated cyclization reactions. Thioureas bearing an additional N-alkyl substituent such as (V) are unable to afford O-alkylation products due to the hindered formation of carbodiimide intermediates.

RX(4) OF 8 A ==> D



I



IV

RX(4) RCT I, 582417RGT 1179 (98-59-9), TosCl1159 (1310-73-2), NaOH

SOL 206 (109-99-9), THF

PRO IV, 582418

T 25.0 Cel

KW alkylation; O-alkylation; etherification

NTE reaction: I -> IV, example: 1

L47 ANSWER 71 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 200150113 CHEMINFORMRX

TI A Mild Cyclodesulfurization of N-(2-Hydroxyethyl)-N'-phenylthioureas to 2-Phenylamino-2-oxazolines Using TsCl/NaOH.

AU KIM, T. H.; LEE, N.; LEE, G.-J.; KIM, J. N.

CS Fac. Appl. Chem., Chonnam Natl. Univ., Kwangju 500-757, S. Korea

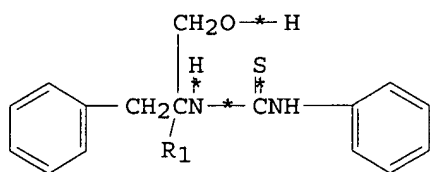
SO Tetrahedron, 57(33), 7137-7141 (2001)

CODEN: TETRAB ISSN: 0040-4020

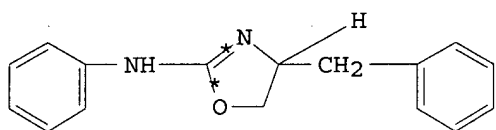
LA English

AB Treatment of thiourea derivatives with TosCl/NaOH leads to oxazolines, thiazolines, and/or imidazolidines depending on the N-substituents. This offers a new entry to the synthesis of 2-phenylamino-2-oxazolines which are of biological interest.

RX(1) OF 10 A ==> B



I



II

YIELD 90.0%

RX(1) RCT I, 721322, (S)-isomer
 RGT 1179 (98-59-9), TosCl
 1159 (1310-73-2), NaOH
 SOL 206 (109-99-9), THF
 222 (7732-18-5), H2O
 PRO II, 846895, (S)-isomer
 YDS 90.0 %
 T 25.0 Cel
 KW alkylation; O-alkylation; etherification
 NTE reaction: (S)-I -> (S)-II, example: 1

147 ANSWER 72 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 200112133 CHEMINFORMRX

TI Ring Closure of N-(2-Hydroxyethyl)-N'-phenylthioureas: One-Pot Synthesis of 2-Phenylaminothiazolines.

AU KIM, T. H.; MIN, J. K.; LEE, G.-J.

CS Fac. Appl. Chem., Chonnam Natl. Univ., Kwangju 500-757, S. Korea

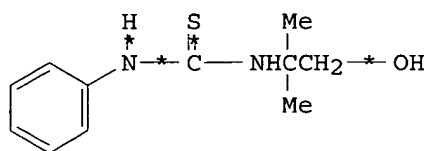
SO Bull. Korean Chem. Soc., 21(9), 919-922 (2000)

CODEN: BKCSDE ISSN: 0253-2964

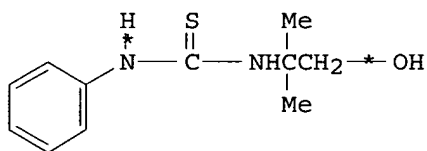
LA English

AB 2-Phenylaminothiazolines (IV) (8 examples) are synthesized in a mild one-pot synthesis by S-cyclization of the corresponding readily available phenylthioureas (III).

RX(4) OF 11 ...2 C ==> I + J

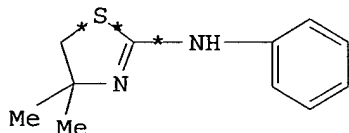
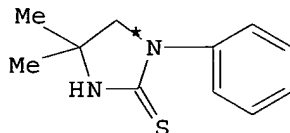


III



III

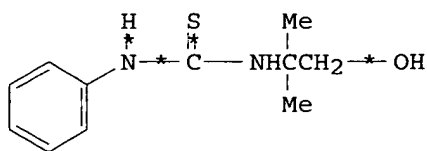
(4) →

IV
YIELD 94.0%V
YIELD 0.0%

RX(4) RCT III, 721315
 RGT 1179 (98-59-9), TosCl
 1159 (1310-73-2), NaOH
 SOL 222 (7732-18-5), H₂O
 206 (109-99-9), THF
 PRO IV, 721318
 V, 797425
 YDS 94.0 %
 T 25.0 Cel
 KW alkylation; S-alkylation; N-alkylation
 NTE reaction: III -> IV + V, example: 1

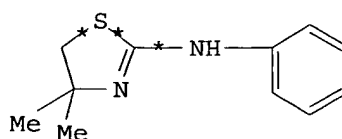
L47 ✓ ANSWER 73 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN
 AN 200005139 CHEMINFORMRX
 TI One-Pot Synthesis of 2-Phenylaminothiazolines from N-(2-Hydroxyethyl)-N'-phenylthioureas.
 AU KIM, T. H.; MIN, J. K.; LEE, G.-J.
 CS Fac. Appl. Chem., Chonnam Natl. Univ., Kwangju 500-757, S. Korea
 SO Tetrahedron Lett., 40(47), 8201-8204 (1999)
 CODEN: TELEAY ISSN: 0040-4039
 LA English
 AB A successful mild synthetic method for 2-phenylaminothiazoles from 1,2-amino alcohols is developed. The readily available thiourea precursors (III) react under one-pot conditions using Tos-Cl in the presence of base.

RX(4) OF 15 ...C ==> I



III

(4) →

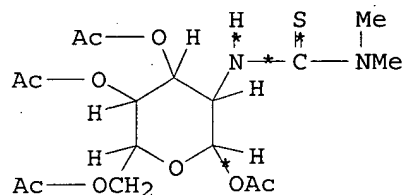
IV
YIELD 94.0%

RX(4) RCT III, 721315
 RGT 1179 (98-59-9), TosCl
 1159 (1310-73-2), NaOH
 SOL 206 (109-99-9), THF
 PRO IV, 721318
 YDS 94.0 %
 T 25.0 Cel
 TIM 0.5 hr
 KW alkylation; S-alkylation
 NTE reaction:III -> IV, example: 1

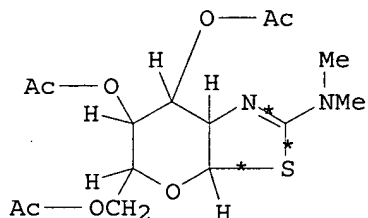
~~L47 ANSWER 74 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN~~
~~AN 199742250 CHEMINFORMRX~~

TI An Allosamizoline/Glucosamine Hybrid NAGase Inhibitor.
 AU KNAPP, S.; KIRK, B. A.; VOCADLO, D.; WITHERS, S. G.
 CS Dep. Chem., Rutgers State Univ. N. J., Piscataway, NJ 08855, USA
 SO Synlett(5), 435-436 (1997)
 CODEN: SYNLES ISSN: 0936-5214
 LA English
 AB Title compound (V) is prepared for structure-activity studies concerning the oxazoline moiety in allosamidin. Compared to the known powerful inhibitor (VI) of jack bean NAGase, the activity of (V) is considerably decreased.

RX(2) OF 6 ...C ==> E...



III



IV
YIELD 71.0%

RX(2) RCT III, 558364, CHIRAL
 RGT 1765 (79271-56-0), Et3Si-O-Tf
 5172 (70955-01-0;69912-79-4;63231-69-6), molecular sieves
 SOL 36 (67-66-3), CHCl3
 PRO IV, 558365, CHIRAL
 YDS 71.0 %
 T 0.0 Cel
 KW alkylation; S-alkylation
 NTE reaction:III* -> IV*

~~L47 ANSWER 75 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN~~

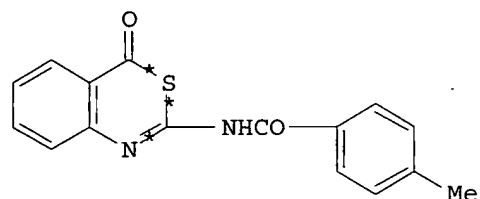
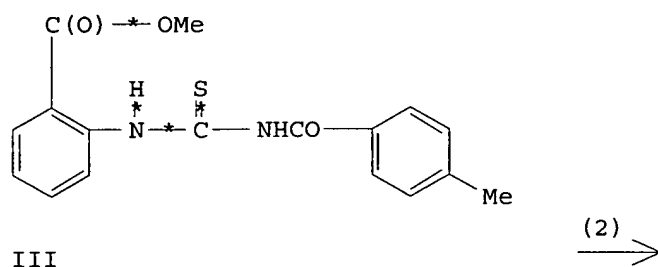
AN 199640158 CHEMINFORMRX
 TI Novel Heterocycles Derived from Substituted Aroylthioureas: Synthesis of 3,1-Benzothiazin-4-ones, Thieno(3,2-d)(1,3)thiazin-4-ones and 1,2,4-Thiadiazolo(2,3-a)(3,1)benzothiazin-5-ones.
 AU GUETSCHOW, M.
 CS Inst. Pharm., Pharm. Chem., Univ. Leipzig, D-04103 Leipzig, Germany
 SO J. Heterocycl. Chem., 33(2), 355-360 (1996)

CODEN: JHTCAD ISSN: 0022-152X

LA English

AB Ring closure reaction of heterocyclic aroylthioureas are investigated. Thus, acidic treatment leads to 3,1-benzothiazinones whereas oxidative ring closure gives thiazoles such as (VII) or the quinazolinedione (IX). Product (XVI) represents a new heterocyclic system.

RX(2) OF 11 ...C ==> E



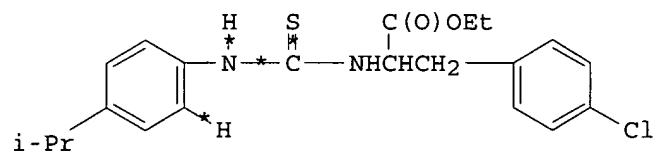
IV
YIELD 80.0%

RX(2) RCT III, 489793
 RGT 198 (7664-93-9), H2SO4
 PRO IV, 489794
 YDS 80.0 %
 T 25.0 Cel
 TIM 48 hr
 KW acylation; S-acylation
 NTE reaction: III -> IV

L47 ANSWER 76 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN
 AN 199434152 CHEMINFORMRX
 TI Benzoxazolamines and Benzothiazolamines: Potent, Enantioselective Inhibitors of Leukotriene Biosynthesis with a Novel Mechanism of Action.
 AU LAZER, E. S.; MIAO, C. K.; WONG, H.-C.; SORCEK, R.; SPERO, D. M.; GILMAN, A.; PAL, K.; BEHNKE, M.; GRAHAM, A. G.; WATROUS, J. M.; HOMON, C. A.; NAGEL, J.; SHAH, A.; GUINDON, Y.; FARINA, P. R.; ADAMS, J.
 CS Dep. Med. Chem., Boehringer Ingelheim Pharm., Inc., Ridgefield, CT 06877, USA
 SO J. Med. Chem., 37(7), 913-923 (1994)
 CODEN: JMCMAR ISSN: 0022-2623
 LA English
 AB Based on (S)-N-(benzothiazol-2-yl)phenylalanine ethyl ester as efficient inhibitor of Ca-ionophore-stimulated leukotriene biosynthesis in human neutrophils, a series of other benzothiazolamine analogues (15 compounds),

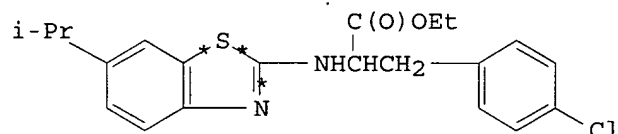
e.g. (IV), and benzoxazoline analogues (55 compounds), e.g. (VIII), (XV), or (XXII), is prepared by structural modification and obtained in racemic or enantiomerically pure form. Hydrophobic substituents in 5-position of the benzoxazole ring and replacement of the phenyl group with a cyclohexyl group in the amino acid moiety improve the inhibitory activity thus leading to the S- enantiomer of (XV) as the most potent derivative. The title compounds are not inhibitors of 5-lipoxygenase, but act at the level of arachidonic acid release.

RX(2) OF 26 ...C ==> E



III

(2) →



IV

YIELD 68.0%

RX(2) RCT III, 329581
 RGT 199 (7791-25-5), SO₂Cl₂
 SOL 35 (108-90-7), PhCl
 PRO IV, 329582
 YDS 68.0 %
 T 0.0 Cel
 KW arylation
 NTE reaction:III -> IV

47 ANSWER 77 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 199352205 CHEMINFORMRX

TI Reactivity of Esters and Nitriles of 2-(3-Acylthioureido)-4,5,6,7-tetrahydrobenzo(b)thiophene-3-carboxylic Acids. Part 1. Acid-Catalyzed Cyclization and Desulfonation Reaction in the Presence of Secondary Amines.

AU PAZDERA, P.; PREISSOVA, I.

CS Dep. Org. Chem., Fac. Nat. Sci., Masaryk Univ., 61137 Brno, Czech Rep.

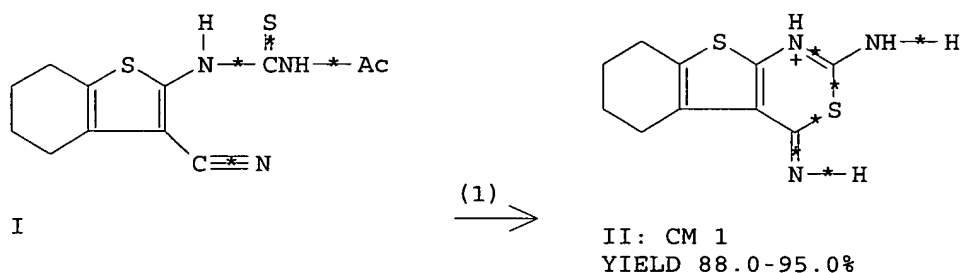
SO Chem. Zvesti, 46(6), 396-405 (1992)

CODEN: CHZVAN ISSN: 0366-6352

LA English

AB The title compounds such as (I) and (V) undergo ring closure on treatment with concentrate sulfuric acid to yield fused tricyclic systems, e. g. (II). With secondary amines, the guanidines (IV) and (VI) are obtained, which can be cyclized to give fused pyrimidines as shown with the formation of (VII).

RX(1) OF 9 A ==> B

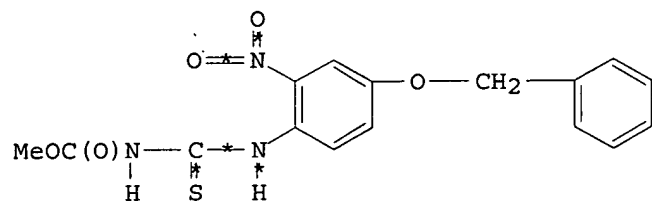
ClO₄⁻

II: CM 2
YIELD 88.0-95.0%

RX(1) RCT I, **282225** (127981-99-1)
 STAGE(1)
 RGT **198** (7664-93-9), H₂SO₄
 T 25.0 Cel
 TIM 48 - 96 hr
 STAGE(2)
 RGT 164 (7601-90-3), HClO₄
 SOL 222 (7732-18-5), H₂O
 T 0.0 - 20.0 Cel
 TIM 2.0 - 3.0 hr
 PRO II, **282226**
 YDS 88.0 - 95.0 %
 KW alkylation; S-alkylation
 NTE reaction:I -> II

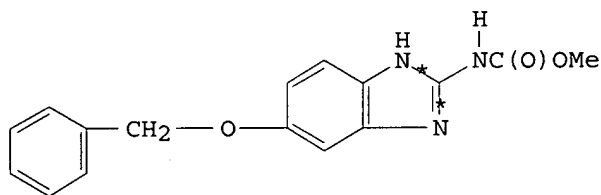
L47 ANSWER 78 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN
 AN 199237151 CHEMINFORMRX
 TI Synthesis, Antineoplastic and Anthelmintic Activities of N-Alkyloxycarbonyl-N'-(4-benzyloxy-2-nitrophenyl)thioureas as Prodrugs of (6-Benzyloxy-1H-benzimidazol-2-yl)carbamic Acid Ester.
 AU BERA, T.; BELSARE, D. P.
 CS Sai Udyan Apartment, Mangal Nagar, Nashik 422 002, India
 SO Indian J. Chem., Sect. B, 31(6), 370-372 (1992)
 CODEN: IJSBDB ISSN: 0376-4369
 LA English
 AB Biological activities of the compounds (VI) and (VII) are evaluated against Ehrlich ascites carcinoma, ascaris and hymenolepsis infected animals. The methyl carbamates (VIa) and (VIIa) cause 90 to 100% elimination of ascaris and hymenolepsis species while the ethyl carbamates (VIb) and (VIIb) show poor activity. Fermentation of (VIa) with E. coli results in the formation of the cyclic product (VIIa). Compound (VIa) cannot be considered as a prodrug of (VIIa) as expected, because the former is not inert and is rather more active than the latter.

RX(4) OF 11 ...H ==> N



VI

(4) →



VII

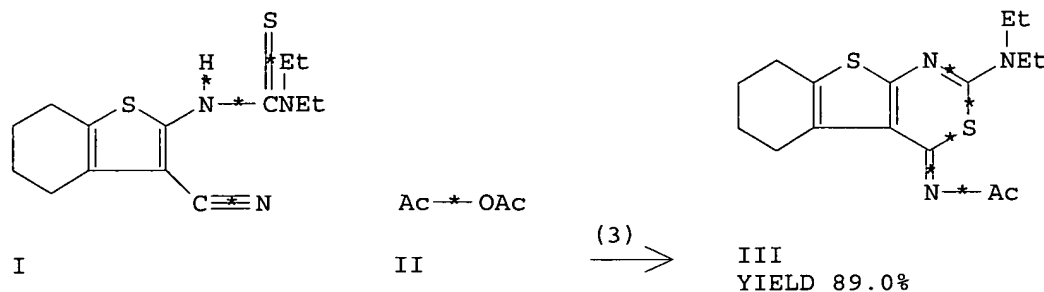
YIELD 96.0%

RX(4) RCT VI, 67512 (142646-10-4)
 RGT 1218 (7775-14-6), Na2S2O4
 SOL 123 (67-56-1), MeOH
 PRO VII, 67514 (54029-21-9)
 YDS 96.0 %
 T.KW REFLUX
 KW alkylation; N-alkylation
 NTE reaction: VI -> VII, example: 1
 CMT Ratio = 1:9 for products 1,2

L47 ANSWER 79 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 199236203 CHEMINFORMRX
 TI Polycyclic Azines with Heteroatoms in the 1- and 3-Position. Part 27.
 One-Pot Synthesis of 4-Acylimino-2-aminothieno(2,3-d)(1,3)thiazines from
 2-Thioureidothiophene-3-carbonitriles.
 AU GUETSCHOW, M.; LEISTNER, S.; PINK, M.
 CS Lehrstuhl Pharm. Chem., Univ. Leipzig, O-7010 Leipzig, Fed. Rep. Ger.
 SO J. Heterocycl. Chem., 29(2), 279-282 (1992)
 CODEN: JHTCAD ISSN: 0022-152X
 LA English
 AB The reaction of the title carbonitriles (I) with propionic anhydride
 proceeds analogously to the reaction described in the scheme. The
 structure of the product (IIIb) is confirmed by X-ray analysis.

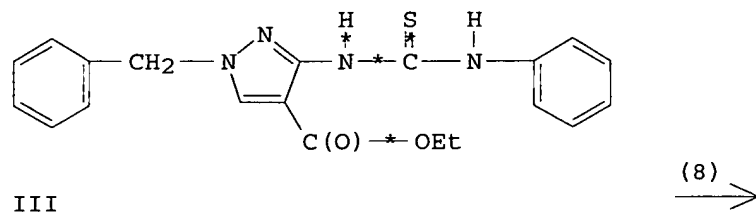
RX(3) OF 3 G + B ==> H

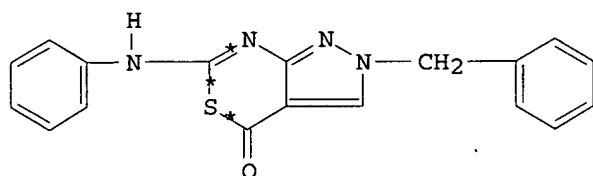


RX(3) RCT I, 66633 (128342-47-2)
 II, 4 (108-24-7)
 RGT 198 (7664-93-9), H₂SO₄
 PRO III, 66634
 YDS 89.0 %
 TIM 96 hr
 KW acetylation; acylation; N-acylation; alkylation; S-alkylation
 NTE reaction: I (II) -> III, example: 3
 CMT #E0100: (diastereom. mix.)

L47 ANSWER 80 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN
 AN 199207162 CHEMINFORMRX
 TI New Pyrazole Derivatives. Part 4. Preparation and Cyclization of Some
 Acceptor-Substituted N-(Pyrazol-3-yl)-thioureas.
 AU EISENACHER, TH.; PECH, R.; BOEHM, R.
 CS Fachbereich Pharm., Martin-Luther-Univ. Halle-Wittenberg, O-4050 Halle/
 S., Fed. Rep. Ger.
 SO J. Prakt. Chem., 333(3), 437-446 (1991)
 CODEN: JPCEAO ISSN: 0021-8383
 LA German
 AB The title compounds (III) (25 examples) can also be obtained by
 interaction of (I) with thiophosgene and reaction of the 2-
 isothiocyantopyrazoles thus obtained with amines. Cyclization with NaOH
 in methanol leads to thiones of type (IV) (10 examples) which, on
 alkylation, form 6-alkylthio derivatives. Acid-initiated cyclization gives
 thiazin-4-ones such as (V) (9 examples).

RX(8) OF 10 ...F ==> R





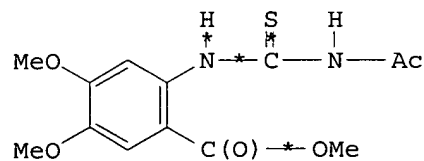
V
YIELD 14.0%

RX(8) RCT III, 19421 (36074-77-8)
RGT 198 (7664-93-9), H₂SO₄
PRO V, 19429 (136603-40-2)
YDS 14.0 %
KW acylation; S-acylation
NTE reaction:IIIb -> V

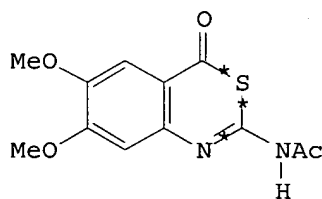
~~47 ANSWER 81 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ-CHEMIE-on-STN~~

AN 199147198 CHEMINFORMRX
TI Polycyclic Azines with Heteroatoms in Position 1 and 3. Part 30. Synthesis of 6,7-Dimethoxy-Substituted 3,1-Benzothiazin-4-ones.
AU GUETSCHOW, M.; HEINECKE, K.; THIEL, W.; LEISTNER, S.
CS Lehrstuhl Pharm. Chem., Sect. Biowiss., Univ., O-7010 Leipzig, Fed. RepGer.
SO Arch. Pharm. (Weinheim, Ger.), 324(7), 465-466 (1991)
CODEN: ARPMAS ISSN: 0365-6233
LA German
AB The dimethoxy-ortho-aminobenzoate (I) reacts with the isothiocyanates (II) to form the N-acylthioureas (III). These are treated with concentrated sulfuric acid under various conditions to undergo cyclocondensation, yielding the aminobenzothiazinone derivatives (IV) - (VII).

RX(3) OF 10 ...C ==> H



III



IV
YIELD 46.0%

RX(3) RCT III, 195853 (134241-04-6)
RGT 198 (7664-93-9), H₂SO₄
PRO IV, 195855 (134241-03-5)
YDS 46.0 %
T 25.0 Cel
TIM 3.0 hr
KW acylation; S-acylation
NTE reaction:IIIa -> IV
CMT Ratio = 1:1 for products 1,2

L47 ANSWER 82 OF 82 CHEMINFORMRX COPYRIGHT 2007 FIZ CHEMIE on STN

AN 199124178 CHEMINFORMRX

TI Polycyclic Azines. Part 25. 2-Amino-3,1-benzothiazin-4-ones: Synthesis, Dimroth Rearrangement to Quinazolin-4(3H)-on-2(1H)-thiones, and MS/MS-Fragmentation.

AU LEISTNER, S.; GUETSCHOW, M.; STACH, J.

CS Sekt. Biowiss., Karl-Marx-Univ. Leipzig, Ber. Chem. Biol. Akt. Verb., O-7010 Leipzig, Germany

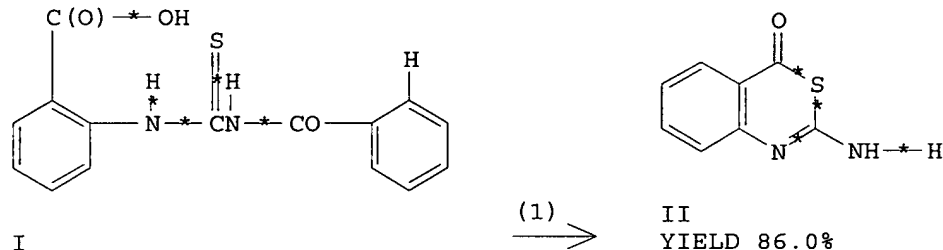
SO Arch. Pharm. (Weinheim, Ger.), 323(10), 857-862 (1990)

CODEN: ARPMAS ISSN: 0365-6233

LA German

AB The N-benzoylthioureas (I) are cyclized in concentrated sulfuric acid to form the benzothiazinones (II) or (III) depending on the reaction conditions. Cyclization of (I) in the presence of a base yields the 2-thioxo-4-quinazolinones (IV). (IVa) is also obtained by Dimroth rearrangement of the benzothiazinone (IIa). The mass spectrometric fragmentation patterns of (II) - (IV) are discussed.

RX(1) OF 11 A ==> B...



RX(1) RCT I, 153740 (13277-24-2)
RGT 198 (7664-93-9), H₂SO₄
PRO II, 153741 (131357-73-8)
YDS 86.0 %
T 100.0 Cel
TIM 4.0 hr
KW acylation; S-acylation
NTE reaction:I -> II, example: 1

INVENTOR SEARCH

Loewe 10/840;105

1/310

01/17/2007

=> d que nos l43

L4 STR
L6 118553 SEA FILE=REGISTRY SSS FUL L4
L10 11576 SEA FILE=HCAPLUS ABB=ON PLU=ON L6
L40 QUE ABB=ON PLU=ON HEINELT, U?/AU
L41 QUE ABB=ON PLU=ON LANG, H?/AU
L43 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND (L40 OR L41)

=> d his l46

(FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 10:49:42 ON 17 JAN 2007)

L46 1 S L45 AND L40-L41

=> d que nos l46

L4 STR
L6 118553 SEA FILE=REGISTRY SSS FUL L4
L40 QUE ABB=ON PLU=ON HEINELT, U?/AU
L41 QUE ABB=ON PLU=ON LANG, H?/AU
L44 84 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND (MEDLINE OR EMBASE OR BIOSIS)/LC
L45 5270 SEA L44
L46 1 SEA L45 AND (L40 OR L41)

=> dup rem l43 l46

FILE 'HCAPLUS' ENTERED AT 11:11:57 ON 17 JAN 2007
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FILE 'MEDLINE' ENTERED AT 11:11:57 ON 17 JAN 2007

PROCESSING COMPLETED FOR L43

PROCESSING COMPLETED FOR L46

L48 16 DUP REM L43 L46 (1 DUPLICATE REMOVED)
ANSWERS '1-16' FROM FILE HCAPLUS

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 11:12:12 ON 17 JAN 2007
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jan 12, 2007 (20070112/UP).

=> d ibib ed ab 1-16

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L48 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 1989:225220 HCAPLUS

DOCUMENT NUMBER: 110:225220

TITLE: Piretanide-dextran and piretanide-polyethylene glycol
interact with high affinity with the sodium chloride
potassium cotransporter in the thick ascending limb of

the loop of Henle
 AUTHOR(S): Nitschke, R.; Schlatter, E.; Eidelman, O.; Lang, H. J.; Englert, H. C.; Cabantchik, Z. I.; Greger, R.
 CORPORATE SOURCE: Physiol. Inst., Univ. Freiburg, Freiburg, D-7800, Fed. Rep. Ger.
 SOURCE: Pfluegers Archiv (1989), 413(5), 559-61
 CODEN: PFLABK; ISSN: 0031-6768
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 25 Jun 1989
 AB High-mol.-weight polyethylene glycol and dextran derivs. of piretanide bound reversibly and with high affinity to the Na⁺ 2Cl⁻ K⁺ cotransporter in isolated rabbit thick ascending limb of the loop of Henle. The compds. had only a weak diuretic effect in rat and were not metabolized in the kidney. It can be concluded that the binding site for piretanide diuretics on the Na⁺ 2Cl⁻ K⁺ cotransporter must be exposed on the surface of the luminal cell membrane.

~~148~~ ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:260072 HCAPLUS
 DOCUMENT NUMBER: 142:316840
 TITLE: Preparation of thienoimidazoles and related compounds as hydrogen ion-sodium exchanger (NHE-3) inhibitors
 INVENTOR(S): Lang, Hans-jochen; Heinelt, Uwe; Wirth, Klaus; Licher, Thomas
 PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005026173	A1	20050324	WO 2004-EP9836	20040903
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10341240	A1	20050407	DE 2003-10341240	20030908
US 2005075385	A1	20050407	US 2004-926118	20040825
AU 2004272225	A1	20050324	AU 2004-272225	20040903
CA 2537695	A1	20050324	CA 2004-2537695	20040903
EP 1664058	A1	20060607	EP 2004-764791	20040903
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1845926	A	20061011	CN 2004-80025656	20040903
NO 2006001559	A	20060406	NO 2006-1559	20060406

PRIORITY APPLN. INFO.:

DE 2003-10341240 A 20030908
US 2004-537738P P 20040120
WO 2004-EP9836 W 20040903

ED Entered STN: 25 Mar 2005

AB Title compds. I [R1 = (un)substitutyed Ph, 3-thienyl; R2, R3 = H, halo, Me, etc.; R4 = H, Me, Et, etc.] and their pharmaceutically acceptable salts were prepared For example, MeI mediated cyclization of thiourea II, e.g., prepared from 3,4-diaminothiophene dihydrochloride and 2,6-dichlorophenylisothiocyanate, afforded the hydrochloride salt of thienoimidazole III. In NHE-3 inhibition assays, 5-examples of compds. I exhibited IC50 values ranging from 0.15-6.51 μ M, e.g., the IC50 value of thienoimidazole III was 0.22 μ M. Compds. I are claimed to be useful for the treatment of breathing disorders.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

U48 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

My application

ACCESSION NUMBER: 2004:1036708 HCAPLUS

DOCUMENT NUMBER: 142:23282

TITLE: Process for synthesizing heterocyclic compounds by reaction of diamines, amino alcohols, or amino thioalcohols with isothiocyanates and cyclization of thiourea intermediates

INVENTOR(S): Heinelt, Uwe; Lang, Hans-Jochen

PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany

SOURCE: U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004242560	A1	20041202	US 2004-840105	20040506
DE 10323701	A1	20041223	DE 2003-10323701	20030522
AU 2004240716	A1	20041202	AU 2004-240716	20040510
CA 2526646	A1	20041202	CA 2004-2526646	20040510
WO 2004103976	A2	20041202	WO 2004-EP4955	20040510
WO 2004103976	A3	20050210		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1631552	A2	20060308	EP 2004-731903	20040510
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, TR, BG, CZ, EE, HU, PL, SK			
BR 2004010565	A	20060620	BR 2004-10565	20040510
CN 1795178	A	20060628	CN 2004-80014178	20040510
NO 2005005991	A	20060214	NO 2005-5991	20051216

PRIORITY APPLN. INFO.:

DE 2003-10323701 A 20030522
US 2003-507143P P 20030930
WO 2004-EP4955 W 20040510

OTHER SOURCE(S): MARPAT 142:23282

ED Entered STN: 03 Dec 2004

AB The invention provides the process for synthesizing heterocyclic compds. of formula (I) [X = S, O, NR₅ (wherein R₅ = H, C1-4 alkyl); m, o = 0, 1, 2; A = each (un)substituted Ph, naphthyl, or heteroaryl; R10-R17 = H, F, partially or fully fluorinated C1-4 alkyl; or R14 and R16 together are a bond, and R15 and R17, together with the two carbon atoms to which they are bonded, form an aromatic six-membered carbocycle, in which one or two carbon atoms may be replaced by nitrogen, or a thiophene ring, wherein the aromatic six-membered carbocycle and the thiophene ring is optionally substituted; wherein, either (i) A is an aromatic ring system, or (ii) the ring formed from R15 and R17 is an aromatic system and m is zero, or (iii) each of A and the ring formed from R15 and R17 is an aromatic ring system] and their tautomers and their salts. In the process, an isothiocyanate of A-NCS (A = same as above) is initially reacted with a primary amine of formula (II) (R = H; m, o, X, R10-R17= same as above) to give a thiourea of formula II [R = A-NH-C(S)]. Subsequently, the thiourea II [R = A-NH-C(S)] is converted to the corresponding heterocycle I using a base and a sulfonyl chloride. Thus, a solution of Ph isothiocyanate (500 mg) in absolute THF (6 mL) was added dropwise over 20 min under argon to a solution of ethylenediamine (5.56 g) in absolute THF (6 mL) and the reaction mixture was treated with H₂O, acidified with 10% HCl, and extracted with EtOAc to give 50 mg 1-(2-aminoethyl)-3-phenylthiourea (III). III (50 mg) was dissolved in THF (1.5 mL) under argon, admixed with a solution of NaOH (25.6 mg) in H₂O (0.6 mL), and treated dropwise with a solution of p-toluenesulfonyl chloride (53.7 mg) in THF within 5 min. and the reaction mixture was stirred for 0.5 h to give, after workup and chromatog. purification, 20 mg 2-(phenylimino)imidazolidine.

L48 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:792335 HCAPLUS

DOCUMENT NUMBER: 141:410834

TITLE: A convenient method for the synthesis of 2-amino substituted aza-heterocycles from N,N'-disubstituted thioureas using TsCl/NaOH

AUTHOR(S): Heinelt, Uwe; Schultheis, Daniela; Jaeger, Siegfried; Lindenmaier, Marion; Pollex, Annett; Beckmann, Henning S. G.

CORPORATE SOURCE: Chemistry, Aventis, Frankfurt, 65926, Germany

SOURCE: Tetrahedron (2004), 60(44), 9883-9888

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:410834

ED Entered STN: 29 Sep 2004

AB P-Toluenesulfonyl chloride (TsCl)/NaOH has been introduced as reagent combination for the synthesis of 2-aminooxazolidines or 2-aminothiazolidines from N-(2-hydroxyethyl)thioureas, but its general application in heterocycle synthesis has not been investigated. In this paper the convenient and efficient synthesis of a variety of 2-amino-substituted 1-aza-3-(aza, oxa or thia) heterocycles of different substitution and ring sizes is described. The application of polymer-supported TsCl facilitates work-up and renders the reaction

conditions very suitable for parallel or robot synthesis.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L48 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:972070 HCAPLUS

DOCUMENT NUMBER: 140:27822

TITLE: Preparation of N-thiophenyl-1H-benzimidazol-2-amines
and related compounds as NHE-3 sodium-proton exchanger
inhibitors

INVENTOR(S): Lang, Hans-Jochen; Heinelt, Uwe;
Hofmeister, Armin; Wirth, Klaus; Gekle, Michael;
Bleich, Markus

PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE: PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003101984	A1	20031211	WO 2003-EP5465	20030526
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10224892	A1	20031218	DE 2002-10224892	20020604
CA 2488242	A1	20031211	CA 2003-2488242	20030526
AU 2003273553	A1	20031219	AU 2003-273553	20030526
EP 1513834	A1	20050316	EP 2003-740148	20030526
EP 1513834	B1	20060315		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003011548	A	20050412	BR 2003-11548	20030526
CN 1659163	A	20050824	CN 2003-812846	20030526
JP 2005533038	T	20051104	JP 2004-509675	20030526
AT 320425	T	20060415	AT 2003-740148	20030526
PT 1513834	T	20060630	PT 2003-740148	20030526
ES 2258722	T3	20060901	ES 2003-3740148	20030526
NZ 536970	A	20060929	NZ 2003-536970	20030526
US 2004006119	A1	20040108	US 2003-448851	20030530
US 7049333	B2	20060523		
ZA 2004009095	A	20050510	ZA 2004-9095	20041110
NO 2004005504	A	20050125	NO 2004-5504	20041216
US 2006160873	A1	20060720	US 2006-385331	20060321
PRIORITY APPLN. INFO.:			DE 2002-10224892	A 20020604
			US 2002-415788P	P 20021003
			WO 2003-EP5465	W 20030526
			US 2003-448851	A1 20030530

OTHER SOURCE(S): MARPAT 140:27822

ED Entered STN: 14 Dec 2003

AB Title compds. I [R1, R2 = H, halo, CN, etc.; R3 = H, CH3, halo, etc.; R4 = H, cycloalkyl, alkenyl, etc.; R5, R6 = H, or together as a bond (sic); R7, R8 = alkyl, alkenyl, alkynyl, etc.] and their pharmaceutically acceptable salts were prepared For example, N-chlorosuccinimide mediated chlorination of thiophene II, e.g., prepared from 3-amino-2-thiophenecarboxylic acid Me ester in 7-steps, afforded the hydrochloride salt of benzimidazolamine III. In NHE-3 sodium-proton exchanger inhibition assays, 12-examples of compds. I exhibited IC50 values ranging from 0.12-1.59 μ M, e.g., the IC50 value of benzimidazolamine III hydrochloride was 0.14 μ M. Compds. I are claimed useful for the treatment of breathing disturbances, ischemic and/or reperfusion events, etc.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ✓ ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:511142 HCAPLUS

DOCUMENT NUMBER: 139:85344

TITLE: Preparation of 1H-imidazol-2-amines as sodium hydrogen exchanging transport protein-3 (NHE3) inhibitors

INVENTOR(S): Heinelt, Uwe; Lang, Hans-Jochen;
Hofmeister, Armin; Wirth, Klaus

PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053434	A1	20030703	WO 2002-EP13921	20021209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10163239	A1	20030710	DE 2001-10163239	20011221
CA 2470856	A1	20030703	CA 2002-2470856	20021209
AU 2002361990	A1	20030709	AU 2002-361990	20021209
EP 1461034	A1	20040929	EP 2002-796586	20021209
EP 1461034	B1	20061122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002015154	A	20041019	BR 2002-15154	20021209
CN 1606440	A	20050413	CN 2002-825817	20021209
JP 2005516947	T	20050609	JP 2003-554191	20021209
US 2003187045	A1	20031002	US 2002-323799	20021220
NO 2004003009	A	20040715	NO 2004-3009	20040715
US 2005004198	A1	20050106	US 2004-892994	20040716

PRIORITY APPLN. INFO.:

DE 2001-10163239 A 20011221
US 2002-353518P P 20020201
WO 2002-EP13921 W 20021209
US 2002-323799 B1 20021220

OTHER SOURCE(S): MARPAT 139:85344

ED Entered STN: 04 Jul 2003

AB Title compds. I [R1, R2 = CN, alkyl, alkenyl, etc.; R3 = halo, alkyl, alkenyl, etc.; R4, R5, R6 = H, halo, alkyl, etc.; R7 = H, halo, alkyl, etc.] and their pharmaceutically acceptable salts were prepared For example, condensation of trans-2,5-dimethylhexan-3,4-diamine and 2,6-dichlorophenylisothiocyanate, followed by DCC mediated cyclization, afforded claimed 1H-imidazol-2-amine II hydrochloride in a one-flask reaction scheme. In sodium hydrogen exchanging transport protein-3 inhibition assays, 3-examples of compds. I exhibited IC50 values ranging from 1.1-19 μ M, e.g., the IC50 value of 1H-imidazol-2-amine II was 1.1 μ M. Compds. I are claimed useful for the treatment of ischemia and lipid metabolic diseases.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L48~~ ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:449660 HCAPLUS

DOCUMENT NUMBER: 137:33293

TITLE: Preparation of 2-anilinobenzimidazoles as inhibitors of Na⁺/H⁺ exchanger (NHE3)

INVENTOR(S): Hofmeister, Armin; Heinelt, Uwe; Lang, Hans-Jochen; Bleich, Markus; Wirth, Klaus; Gekle, Michael

PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany

SOURCE: PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002046169	A1	20020613	WO 2001-EP13586	20011122
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10060292	A1	20020620	DE 2000-10060292	20001205
CA 2430412	A1	20020613	CA 2001-2430412	20011122
AU 200219135	A	20020618	AU 2002-19135	20011122
EE 200300193	A	20030815	EE 2003-193	20011122
EP 1341770	A1	20030910	EP 2001-999563	20011122
EP 1341770	B1	20060614		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2001015936	A	20031028	BR 2001-15936	20011122

JP 2004517086	T	20040610	JP 2002-547908	20011122
HU 200400967	A2	20040830	HU 2004-967	20011122
NZ 526250	A	20041126	NZ 2001-526250	20011122
RU 2272031	C2	20060320	RU 2003-120069	20011122
AT 329906	T	20060715	AT 2001-999563	20011122
US 2002132842	A1	20020919	US 2001-28	20011204
US 6686384	B2	20040203		
US 2003191170	A1	20031009	US 2003-441124	20030520
US 6958357	B2	20051025		
ZA 2003003932	A	20040415	ZA 2003-3932	20030521
NO 2003002490	A	20030722	NO 2003-2490	20030602
IN 2003CN00855	A	20050422	IN 2003-CN855	20030602
PRIORITY APPLN. INFO.:			DE 2000-10060292	A 20001205
			WO 2001-EP13586	W 20011122
			US 2001-28	A3 20011204

OTHER SOURCE(S): MARPAT 137:33293

ED Entered STN: 14 Jun 2002

AB Title compds. [I; R1-R5 = F, Cl, Br, I, cyano, OH, (fluorinated) alkyl, cycloalkyl, oxoalkyl, etc.; R6-R9 = H, F, Cl, Br, I, cyano, OH, (fluorinated) alkyl, cycloalkyl, alkoxy, etc.] and salts thereof were prepared. Thus, 1-(2-amino-6-hydroxyphenyl)-3-(2,6-dichlorophenyl)thiourea (preparation given) in EtOH was refluxed with MeI for 8 h to give 47% 2-[(2,6-dichlorophenyl)amino]-4-hydroxy-1H-benzimidazole hydrochloride. The latter inhibited NHE3 with IC50 = 0.47 μ M.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

148 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:607388 HCAPLUS

DOCUMENT NUMBER: 133:207886

TITLE: Preparation of alkyliminoindanothiazoles and analogs as anorectic agents

INVENTOR(S): Jaehne, Gerhard; Geisen, Karl; Lang, Hans-jochen; Bickel, Martin

PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany

SOURCE: Ger. Offen., 16 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19908536	A1	20000831	DE 1999-19908536	19990226
CA 2364902	A1	20000908	CA 2000-2364902	20000205
WO 2000051996	A1	20000908	WO 2000-EP926	20000205
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1157013	A1	20011128	EP 2000-906286	20000205

EP 1157013 B1 20041208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO
BR 2000008559 A 20011218 BR 2000-8559 20000205
JP 2002538149 T 20021112 JP 2000-602223 20000205
AU 765300 B2 20030911 AU 2000-28022 20000205
AU 2000028022 A 20000921
AT 284394 T 20041215 AT 2000-906286 20000205
PT 1157013 T 20050228 PT 2000-906286 20000205
ES 2232425 T3 20050601 ES 2000-906286 20000205
US 6207689 B1 20010327 US 2000-500464 20000209
US 6288093 B1 20010911 US 2000-697151 20001027
US 2001011096 A1 20010802 US 2001-774053 20010131
US 6288094 B2 20010911
ZA 2001006441 A 20020213 ZA 2001-6441 20010806
HK 1042299 A1 20041210 HK 2002-104046 20020531
PRIORITY APPLN. INFO.: DE 1999-19908536 A 19990226
WO 2000-EP926 W 20000205
US 2000-500464 A3 20000209

OTHER SOURCE(S): MARPAT 133:207886

ED Entered STN: 31 Aug 2000

AB Title compds. [I; R1 = 1 or 2 of halo, alkyl, alkoxy, acyl, etc.; R2,R3 = (carboxy)alkyl, CH2Ph, pyridinyl(alkyl), etc.; R2R3 = (CH2)2-4 or CH2CMe2; Z = O, S, CH2, CHPh; Z1 = bond, CH2, CH2CH2] were prepared. Thus, 2-bromo-5-chloro-1-indanone was cyclocondensed with (MeHN)2CS and the product treated with HOAc to give title compound II.HBr. Data for biol. activity of I were given.

L48 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:488488 HCAPLUS

DOCUMENT NUMBER: 115:88488

TITLE: Macromolecular conjugates of transport inhibitors: new tools for probing topography of anion transport proteins

AUTHOR(S): Eidelman, Ofer; Yanai, Peter; Englert, Heimer C.; Lang, Hans G.; Greger, Rainer; Cabantchik, Z. Ioav

CORPORATE SOURCE: Inst. Life Sci., Hebrew Univ., Jerusalem, 91904, Israel

SOURCE: American Journal of Physiology (1991), 260(5, Pt. 1), C1094-C1103

CODEN: AJPHAP; ISSN: 0002-9513

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 06 Sep 1991

AB Macromol.-conjugated, water-soluble, membrane-impermeant compds. were designed and assessed as topol. probes for chloride-transporting agencies. The novel compds. were derivs. of either disulfonic stilbene (DS) and benzylaminoethylsulfonate (BS), classical inhibitors of erythrocyte chloride-bicarbonate exchange, or of phenylanthranilates (PA), high-affinity blockers of epithelial chloride channels. Covalent reactive derivs. of various DS, BS, and PA were synthesized and coupled either directly to polyethylene glycol or via spacer arms of different lengths to dextrans. The macromol. conjugates were demonstrably inhibitory to red blood cell anion exchange when the ligands were appropriately coupled: inhibitory efficacy strongly depended on the chemical structure of the coupled ligand and the spacer length between the inhibitory moiety and the

macromol. Mechanistic studies indicated that impermeant DS and PA derivs. acted exofacially on sites, which although different in their affinity for chloride, shared geog. proximity. BS derivs. were unique in that they affected transport from either surface. The results suggest asym. aqueous access routes leading to the functional domain of the anion transporter from either membrane surface.

L48/ ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:651434 HCAPLUS

DOCUMENT NUMBER: 115:251434

TITLE: Different types of blockers of the intermediate-conductance outwardly rectifying chloride channel in epithelia

AUTHOR(S): Tilmann, M.; Kunzelmann, K.; Froebe, U.; Cabantchik, I.; Lang, H. J.; Englert, H. C.; Greger, R.

CORPORATE SOURCE: Physiol. Inst., Albert-Ludwigs-Univ., Freiburg, W-7800, Germany

SOURCE: Pfluegers Archiv (1991), 418(5), 556-63
CODEN: PFLABK; ISSN: 0031-6768

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 14 Dec 1991

AB Epithelial Cl⁻ channels can be blocked by various inhibitors that show considerable differences in their mol. structure. In the present patch-clamp study, different blockers of 1 type of epithelial Cl⁻ channel were compared with respect to their inhibitory potency. The blockers were applied to excised inside-out or outside-out-oriented membrane patches of cultured HT29 colon carcinoma and respiratory epithelial cells (REC) containing the outwardly rectifying intermediate-conductance (ICOR) Cl⁻ channel. Four types of inhibitory compds. were tested: stilbene disulfonate derivs., indanyloxyacetic acid, amidine, and aryl-aminobenzoates. The concns. for half-maximal inhibition (IC₅₀) for the different channel blockers were (μmol/L): 4-acetamido-4-isothiocyanatostilbene-2,2'-disulfonic acid 100; 4,4'-diisothiocyanatostilbene-2,2'-disulfonic acid 80; indanyloxyacetic acid 9; 4,4'-dinitrostilbene-2,2'-disulfonic acid 8; amidine 8, and 5-nitro-2-(3-phenylpropylamino)benzoate (NPPB) 0.9. All compound, when applied to the cytosolic side of the channel, induced a flicker-type block of the ICOR Cl⁻ channel at lower concns. and a complete channel inhibition at higher concns. The inhibitory potency of NPPB was much higher when it was added to the external surface of the channel in outside-out-oriented membrane patches. At 1 μmol/L the inhibition was complete. All blocker effects were fully reversible. The probe with the highest affinity (NPPB) and a closely related compound 5-nitro-2-(3-phenylethylamino)-benzoate (NPEB) were used to construct macromol. probes by linking these blockers to aminopolyethylene glycol (PEG) or aminoethyl-O-dextran (5 kilodaltons). These macromol. NPPB and NPEB derivs. inhibited the ICOR Cl⁻ channels only from the outside but had no effect on the cytosolic side. In the case of PEG-NPPB, and IC₅₀ of 30 nmol/L was determined in outside-out patches. The data indicate that the interaction site for arylaminobenzoates is accessible from the outer aspects of the Cl⁻ channel facing the extracellular medium. The macromol. probes of arylaminobenzoates have affinities to the Cl⁻ channel very similar to those of resp. parent compound

L48/ ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:72082 HCAPLUS

DOCUMENT NUMBER: 98:72082
 TITLE: Thiazoline derivatives, their use and their pharmaceutical preparations
 INVENTOR(S): Lang, Hans Jochen; Seuring, Bernhard; Granzer, Ernold
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Eur. Pat. Appl., 45 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 55458	A2	19820707	EP 1981-110677	19811222
EP 55458	A3	19821020		
EP 55458	B1	19850213		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DE 3049460	A1	19820729	DE 1980-3049460	19801230
AT 11778	T	19850215	AT 1981-110677	19811222
ES 508293	A1	19830401	ES 1981-508293	19811223
FI 8104175	A	19820701	FI 1981-4175	19811228
JP 57134472	A	19820819	JP 1981-210093	19811228
US 4421757	A	19831220	US 1981-335149	19811228
IL 64653	A	19850929	IL 1981-64653	19811228
DK 8105811	A	19820701	DK 1981-5811	19811229
NO 8104468	A	19820701	NO 1981-4468	19811229
NO 154551	B	19860707		
ZA 8108968	A	19821124	ZA 1981-8968	19811229
HU 26885	A2	19830928	HU 1981-3984	19811229
HU 184976	B	19841128		
CA 1173836	A1	19840904	CA 1981-393285	19811229
AU 8179068	A	19820708	AU 1981-79068	19811230
AU 542670	B2	19850228		
ES 518272	A1	19830901	ES 1982-518272	19821216
ES 518273	A1	19830901	ES 1982-518273	19821216
ES 518274	A1	19830901	ES 1982-518274	19821216
ES 518271	A1	19840216	ES 1982-518271	19821216
PRIORITY APPLN. INFO.:			DE 1980-3049460	A 19801230
			EP 1981-110677	A 19811222

OTHER SOURCE(S): MARPAT 98:72082

ED Entered STN: 12 May 1984

AB Thiazolines I (R = H, halo, Me; R1 = C1-3 alkyl; R2, R3 = H, halo, C1-4 alkyl or alkoxy; R4, R5 = H, C1-4 alkyl; N R4R5 = saturated ring with ≤6 members; R6 = H, C1-4 acyl), useful in lowering cholesterol in serum very low and low d. lipoproteins with little or no effect on high d. lipoproteins and thus useful in treating atherosclerosis, were prepared by 5 methods. MeNHCSNHC6H4OH-4 and COCl2 in THF gave ClC(NHMe):NC6H4OH-4.HCl which cyclized with 4,3-Cl(Me2NSO)2C6H3COCH2SH in Me2CHOH by treating the mixture successively with NET3 in a little Me2CHOH, CHCl3 with overnight stirring, and AcOH to give II. Rats were treated with 10 mg/kg II per day orally for 7 days; this treatment lowered cholesterol in serum 9%, in the very low d. serum lipoprotein 54%, in low d. lipoprotein 17%, and in high d. serum lipoprotein 4%.

L48 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:425048 HCAPLUS
 DOCUMENT NUMBER: 95:25048
 TITLE: Thiazolidine derivatives or their pharmacologically compatible acid addition salts
 INVENTOR(S): Lang, Hans Jochen; Seuring, Bernhard; Granzer, Ernold
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 110 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2926771	A1	19810115	DE 1979-2926771	19790703
ES 492847	A1	19810216	ES 1980-492847	19800627
ES 492871	A1	19810216	ES 1980-492871	19800627
ES 492872	A1	19810216	ES 1980-492872	19800627
ES 492873	A1	19810216	ES 1980-492873	19800627
ES 492874	A1	19810216	ES 1980-492874	19800627
EP 23964	A1	19810218	EP 1980-103688	19800628
EP 23964	B1	19830216		
R: AT, BE, CH, DE, FR, GB, IT, NL, SE				
AT 2524	T	19830315	AT 1980-103688	19800628
FI 8002094	A	19810104	FI 1980-2094	19800701
US 4346088	A	19820824	US 1980-165218	19800701
DK 8002865	A	19810104	DK 1980-2865	19800702
NO 8001995	A	19810105	NO 1980-1995	19800702
NO 154132	B	19860414		
AU 8060037	A	19810115	AU 1980-60037	19800702
AU 533589	B2	19831201		
ZA 8003979	A	19810624	ZA 1980-3979	19800702
HU 24426	A2	19830228	HU 1980-1643	19800702
HU 182164	B	19831228		
CA 1156240	A1	19831101	CA 1980-355222	19800702
IL 60468	A	19841130	IL 1980-60468	19800702
IL 70114	A	19841130	IL 1980-70114	19800702
JP 56010180	A	19810202	JP 1980-91605	19800703
NO 8404120	A	19810105	NO 1984-4120	19841016
PRIORITY APPLN. INFO.:			DE 1979-2926771	A 19790703
			EP 1980-103688	A 19800628
			IL 1980-60468	A3 19800702

OTHER SOURCE(S): MARPAT 95:25048

ED Entered STN: 12 May 1984

AB Anticholesteremic (no data) thiazolines I (R = H, halogen, alkyl; R1 = alkyl, cycloalkyl, alkenyl; R2-R4 = H, halogen, alkyl, alkoxy, OCH2O, OCH2CH2O, NMe2, NEt2, CF3; R5, R6 = H, alkyl; R7 = H, alkyl, cycloalkyl, allyl, CH2CH2Ph, optionally substituted CH2Ph; NR6R7 = heterocyclic) were prepared. Thus, cyclocondensation of 4,3-Cl(Me2NSO2)C6H3COCH2Br with PhNHCSNHMe gave a thiazolidinol whose dehydration with acid gave I (R = Cl, R1 = R6 = R7 = Me, R2-R5 = H).

L48 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:584487 HCAPLUS

DOCUMENT NUMBER: 87:184487

TITLE: Thiazolidine derivatives
 INVENTOR(S): Lang, Hans Jochen; Muschaweck, Roman
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 68 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2601598	A1	19770721	DE 1976-2601598	19760117
NL 7700259	A	19770719	NL 1977-259	19770112
DK 7700148	A	19770718	DK 1977-148	19770114
FI 7700109	A	19770718	FI 1977-109	19770114
NO 7700123	A	19770719	NO 1977-123	19770114
AU 7721342	A	19780720	AU 1977-21342	19770114
US 4118501	A	19781003	US 1977-759546	19770114
AT 7700189	A	19790615	AT 1977-189	19770114
AT 354440	B	19790110		
IL 51263	A	19791031	IL 1977-51263	19770114
HU 18396	A2	19800628	HU 1977-HO1952	19770114
HU 176109	B	19801228		
CA 1089472	A1	19801111	CA 1977-269714	19770114
BE 850451	A1	19770718	BE 1977-174132	19770117
JP 52093742	A	19770806	JP 1977-3017	19770117
FR 2338269	A1	19770812	FR 1977-1172	19770117
FR 2338269	B1	19810109		
GB 1570912	A	19800709	GB 1977-1749	19770117
US 4156735	A	19790529	US 1978-885643	19780313
AT 7903759	A	19800815	AT 1979-3759	19790522
AT 361473	B	19810310		
AT 7903760	A	19800815	AT 1979-3760	19790522
AT 361474	B	19810310		
PRIORITY APPLN. INFO.:			DE 1976-2601598	A 19760117
			AT 1977-189	A 19770114
			US 1977-759546	A3 19770114

ED Entered STN: 12 May 1984

AB Diuretic (no data) iminothiazolidinols I (R = alkyl, NR1R2 and NR3R4 are amino, R5 = Cl, Br) (>100 compds.) were prepared by cyclocondensation of 3-sulfamoylacetophenones with thioureas. Thus, 4,3-Cl(H2NSO2)C6H3COCH2Br was treated with EtNHCSNMe2 to give I (R = Et, R1 = R2 = Me, R3 = R4 = H, R5 = Cl).

L48 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:453265 HCAPLUS
 DOCUMENT NUMBER: 87:53265
 TITLE: Thiazolidine derivatives
 INVENTOR(S): Lang, Hans Jochen; Muschaweck, Roman
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 54 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2546165	A1	19770428	DE 1975-2546165	19751015
GB 1563323	A	19800326	GB 1976-41722	19761007
NL 7611159	A	19770419	NL 1976-11159	19761008
FI 7602920	A	19770416	FI 1976-2920	19761013
DK 7604640	A	19770416	DK 1976-4640	19761014
NO 7603502	A	19770418	NO 1976-3502	19761014
AU 7618691	A	19780420	AU 1976-18691	19761014
AT 7607655	A	19800115	AT 1976-7655	19761014
AT 358030	B	19800811		
HU 174587	B	19800228	HU 1976-HO1931	19761014
CA 1083581	A1	19800812	CA 1976-263345	19761014
BE 847352	A1	19770415	BE 1976-171562	19761015
SE 7611504	A	19770416	SE 1976-11504	19761015
JP 52051364	A	19770425	JP 1976-124381	19761015
FR 2327778	A1	19770513	FR 1976-31040	19761015
FR 2327778	B1	19781215		
AT 7902625	A	19791215	AT 1979-2625	19790409
AT 357525	B	19800710		

PRIORITY APPLN. INFO.:

DE 1975-2546165	A	19751015
AT 1976-7655	A	19761014

OTHER SOURCE(S): MARPAT 87:53265

ED Entered STN: 12 May 1984

AB Thiazolidines I [R = Me, Et, MeO, EtO, MeNH, BuNH, Pr₂N, cyclopentylamino, cyclohexylamino, piperidino; R₁ = Br, Cl; R₂ = Me, Et, Pr, H₂C:CHCH₂; R₃ = Me, Et, iso-Pr, iso-Bu, H₂C:CHCH₂, Pr, PhCH₂, PhCH₂CH₂, MeCH(OMe)CH₂, cyclohexyl; R₂R₃ = CH₂CH₂, CH₂CH₂CH₂], useful as diuretics (no data), are prepared by cyclocondensation of the appropriate 2,4'-dihaloacetophenone with a suitable 2-thiourea derivative. Thus, reaction of Ac₂O with 3,4-(H₂NSO₂)ClC₆H₃COMe gives 3,4-(AcHNSO₂)ClC₆H₃COMe which is brominated to give 3,4-(AcNHSO₂)ClC₆H₃COCH₂Br (II). Reaction of II with MeNHCSNHMe in EtOH at 45-50° and overnight standing at 20° gives I (R = R₂ = R₃ = Me, R₁ = Cl).

L48 ANSWER 15/OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:423260 HCAPLUS

DOCUMENT NUMBER: 87:23260

TITLE: Thiazolidine derivatives

INVENTOR(S): Lang, Hans Jochen; Muschaweck, Roman

PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 58 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2533821	A1	19770217	DE 1975-2533821	19750729
JP 60000353	B	19850107	JP 1976-527	19760101
NL 7608206	A	19770201	NL 1976-8206	19760723
FI 7602140	A	19770130	FI 1976-2140	19760727
IL 50146	A	19791230	IL 1976-50146	19760727
DK 7603404	A	19770130	DK 1976-3404	19760728

NO 7602625	A	19770201	NO 1976-2625	19760728
AU 498052	B2	19790201	AU 1976-16324	19760728
AT 353267	B	19791112	AT 1976-5555	19760728
AT 7605555	A	19790415		
CA 1077492	A1	19800513	CA 1976-257944	19760728
SE 7608545	A	19770130	SE 1976-8545	19760729
BE 844666	A1	19770131	BE 1976-169365	19760729
JP 52017468	A	19770209	JP 1976-91186	19760729
FR 2319345	A1	19770225	FR 1976-23219	19760729
FR 2319345	B1	19781117		
AT 7901827	A	19811215	AT 1979-1827	19790312
AT 7901828	A	19811215	AT 1979-1828	19790312
AT 7901829	A	19811215	AT 1979-1829	19790312
PRIORITY APPLN. INFO.:			DE 1975-2533821	19750729
			AT 1976-5555	A 19760728

ED Entered STN: 12 May 1984

AB Phenylthiazolidinols [I; R = Me, Et, Me₂CH, Me₂CHCH₂, cyclohexyl, H₂C:CHCH₂, cyclopropyl, Bu, PhCH₂, PhCH₂CH₂, MeCH(OMe)CH₂; R₁ = Me, Et, Me₂CH, cyclohexyl, H₂C:CHCH₂, cyclopropyl, Bu; R₂ = H, Me, Pr; R₃ = Me, Pr, PhCH₂CH₂, PhCH₂, sec-Bu; R₄ = Cl, Me; R₅ = Br, Cl, Me; R₆ = H, Cl], useful as diuretics (no data), are prepared by cyclocondensation of 2-haloacetophenones with thiourea derivs. 3,4,5-Cl₂(H₂NSO₂)C₆H₂CO₂H is converted to the acid chloride which reacts with CH₂N₂ to give 3,4,5-Cl₂(H₂NSO₂)C₆H₂COCHN₂ which is chlorinated to give 3,4,5-Cl₂(H₂NSO₂)C₆H₂COCH₂Cl (II). Reaction of II with EtNHCSNH₂ in MeOH 15 min at 40° gives I (R = R₁ = Et, R₂ = R₃ = R₆ = H, R₄ = R₅ = Cl).

L48 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:463054 HCAPLUS
 DOCUMENT NUMBER: 85:63054
 TITLE: Thiazolidine derivatives
 INVENTOR(S): Lang, Hans J.; Muschaweck, Roman
 PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 149 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2436263	A1	19760212	DE 1974-2436263	19740727
DE 2436263	C2	19830217		
ES 439593	A1	19770616	ES 1975-439593	19750721
IL 47779	A	19790131	IL 1975-47779	19750723
FI 7502131	A	19760128	FI 1975-2131	19750724
FI 61487	B	19820430		
FI 61487	C	19820810		
NL 7508848	A	19760129	NL 1975-8848	19750724
NL 181711	B	19870518		
NL 181711	C	19871016		
ZA 7504772	A	19760630	ZA 1975-4772	19750724
HU 172659	B	19781128	HU 1975-HO1821	19750724
CH 617431	A5	19800530	CH 1975-9689	19750724
DK 7503404	A	19760128	DK 1975-3404	19750725

DK 145626	B	19830103		
DK 145626	C	19830801		
NO 7502636	A	19760128	NO 1975-2636	19750725
NO 144528	B	19810609		
NO 144528	C	19810923		
SE 7508476	A	19760128	SE 1975-8476	19750725
SE 431207	B	19840123		
SE 431207	C	19840503		
DD 121112	A5	19760712	DD 1975-187482	19750725
AU 7583391	A	19770127	AU 1975-83391	19750725
AU 501320	B2	19790614		
AT 7505770	A	19771115	AT 1975-5770	19750725
CA 1054596	A1	19790515	CA 1975-232295	19750725
JP 51054555	A	19760513	JP 1975-90729	19750726
JP 60006945	B	19850221		
BE 831794	A1	19760128	BE 1975-158662	19750728
FR 2282882	A1	19760326	FR 1975-23498	19750728
FR 2282882	B1	19790810		
US 4125614	A	19781114	US 1977-788905	19770419
AT 7707814	A	19800615	AT 1977-7814	19771102
AT 360520	B	19810112		
AT 7707816	A	19800615	AT 1977-7816	19771102
AT 360521	B	19810112		
AT 7707817	A	19800615	AT 1977-7817	19771102
AT 360522	B	19810112		
AT 7707815	A	19800715	AT 1977-7815	19771102
AT 360985	B	19810210		
CH 623316	A5	19810529	CH 1979-10799	19791205
CH 624677	A5	19810814	CH 1979-10797	19791205
CH 624678	A5	19810814	CH 1979-10798	19791205
PRIORITY APPLN. INFO.:			DE 1974-2436263	A 19740727
			CH 1975-9689	A 19750724
			AT 1975-5770	A 19750725
			US 1975-599103	A3 19750725

OTHER SOURCE(S): MARPAT 85:63054

ED Entered STN: 12 May 1984

AB Diuretic and saluretic (no data) iminothiazolidinols I(R = Cl, Br, Me, CHMe₂, H, OMe; R₁ R₂ R₄ = C₁-6 alkyl, C₃-8 cycloalkyl, substituted alkyl, NMe₂; R₃ = H, Et; NR₄R₅ = heterocyclic; R₅ = H, Me, Et, Pr) (133 compds) were prepared by condensing 4,3-R(R₄R₅NSO₂)C₆H₃COCH₂R₆ (R₆ = Cl, Br) with R₁NHCSNHR₂.

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 11:13:55 ON 17 JAN 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jan 12, 2007 (20070112/UP).

=> d his ful

(FILE 'HOME' ENTERED AT 09:20:57 ON 17 JAN 2007)

FILE 'STNGUIDE' ENTERED AT 09:21:11 ON 17 JAN 2007

FILE 'ZCAPLUS' ENTERED AT 09:21:39 ON 17 JAN 2007
E US2004-840105/APPS

L1 FILE 'HCAPLUS' ENTERED AT 09:22:31 ON 17 JAN 2007
1 SEA ABB=ON PLU=ON US2004-840105/APPS
SAVE TEMP L1 LOE105HCAAPP/A

FILE 'STNGUIDE' ENTERED AT 09:22:48 ON 17 JAN 2007
D QUE

FILE 'HCAPLUS' ENTERED AT 09:23:26 ON 17 JAN 2007
D IBIB ED AB IND

FILE 'STNGUIDE' ENTERED AT 09:23:27 ON 17 JAN 2007

FILE 'REGISTRY' ENTERED AT 09:23:56 ON 17 JAN 2007

L2 FILE 'HCAPLUS' ENTERED AT 09:23:59 ON 17 JAN 2007
TRA PLU=ON L1 1- RN : 72 TERMS

L3 FILE 'REGISTRY' ENTERED AT 09:24:01 ON 17 JAN 2007
72 SEA ABB=ON PLU=ON L2
SAVE TEMP LOE105REGAPP/A L3

FILE 'STNGUIDE' ENTERED AT 09:27:09 ON 17 JAN 2007

L4 FILE 'REGISTRY' ENTERED AT 09:28:04 ON 17 JAN 2007
STRUCTURE UPLOADED
D QUE STAT

L5 50 SEA SSS SAM L4
D QUE STAT

FILE 'STNGUIDE' ENTERED AT 09:31:17 ON 17 JAN 2007

L6 FILE 'REGISTRY' ENTERED AT 09:33:06 ON 17 JAN 2007
118553 SEA SSS FUL L4
SAVE TEMP L6 LOE105PSETR/A

L7 FILE 'ZCAPLUS' ENTERED AT 09:34:36 ON 17 JAN 2007
QUE ABB=ON PLU=ON ?CYCLIZ? OR ?CYCLIS? OR (RING (2A) (CLOS?
OR FORM OR FORMING OR FORMS OR FORMATION))
L8 QUE ABB=ON PLU=ON ?CYCLODESUL? OR (CYCLO(W) DESUL?)
L9 QUE ABB=ON PLU=ON CYCLO (W) DE(W) (SULF? OR SULPH?)

L10 FILE 'HCAPLUS' ENTERED AT 09:38:07 ON 17 JAN 2007
11576 SEA ABB=ON PLU=ON L6

FILE 'STNGUIDE' ENTERED AT 09:38:59 ON 17 JAN 2007

L11 FILE 'HCAPLUS' ENTERED AT 09:39:52 ON 17 JAN 2007
2989 SEA ABB=ON PLU=ON L6 (L) RACT+NT/RL

L12 652 SEA ABB=ON PLU=ON L10 (L) (L7 OR L8 OR L9)
L13 591 SEA ABB=ON PLU=ON L11 AND L12

FILE 'STNGUIDE' ENTERED AT 09:41:37 ON 17 JAN 2007

FILE 'HCAPLUS' ENTERED AT 09:42:02 ON 17 JAN 2007
L14 0 SEA ABB=ON PLU=ON L1 NOT L13

FILE 'STNGUIDE' ENTERED AT 09:42:35 ON 17 JAN 2007

FILE 'ZCAPLUS' ENTERED AT 09:43:53 ON 17 JAN 2007
L15 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004 OR MY<2004
OR REVIEW/DT

FILE 'HCAPLUS' ENTERED AT 09:44:52 ON 17 JAN 2007
L16 549 SEA ABB=ON PLU=ON L13 AND L15

FILE 'STNGUIDE' ENTERED AT 09:45:12 ON 17 JAN 2007

FILE 'STNGUIDE' ENTERED AT 09:47:56 ON 17 JAN 2007

FILE 'REGISTRY' ENTERED AT 09:53:41 ON 17 JAN 2007
L17 STRUCTURE UPLOADED
D QUE STAT
L18 50 SEA SSS SAM L17

FILE 'STNGUIDE' ENTERED AT 09:54:36 ON 17 JAN 2007

FILE 'REGISTRY' ENTERED AT 09:58:01 ON 17 JAN 2007
L19 STRUCTURE UPLOADED
D QUE STAT
L20 50 SEA SSS SAM L19

FILE 'STNGUIDE' ENTERED AT 09:58:52 ON 17 JAN 2007

FILE 'REGISTRY' ENTERED AT 09:59:34 ON 17 JAN 2007
L21 5 SEA ABB=ON PLU=ON L6 AND L3
D SCAN
D QUE L6

L22 117457 SEA ABB=ON PLU=ON L6 NOT P/ELS
L23 116772 SEA ABB=ON PLU=ON L22 NOT M/ELS

FILE 'HCAPLUS' ENTERED AT 10:02:13 ON 17 JAN 2007
L24 29 SEA ABB=ON PLU=ON L21

FILE 'STNGUIDE' ENTERED AT 10:02:49 ON 17 JAN 2007

FILE 'HCAPLUS' ENTERED AT 10:03:23 ON 17 JAN 2007
L25 3 SEA ABB=ON PLU=ON L24 AND L13
L26 11035 SEA ABB=ON PLU=ON L23
L27 588 SEA ABB=ON PLU=ON L13 AND L26

FILE 'STNGUIDE' ENTERED AT 10:04:34 ON 17 JAN 2007

FILE 'REGISTRY' ENTERED AT 10:05:23 ON 17 JAN 2007
L28 5457 SEA ABB=ON PLU=ON L6 AND CASREACT/LC

FILE 'STNGUIDE' ENTERED AT 10:05:55 ON 17 JAN 2007

L29 FILE 'CASREACT' ENTERED AT 10:08:32 ON 17 JAN 2007
STRUCTURE UPLOADED
D QUE STAT

L30 50 SEA SSS SAM L29 (494 REACTIONS)
D QUE STAT

FILE 'STNGUIDE' ENTERED AT 10:11:43 ON 17 JAN 2007

L31 FILE 'CASREACT' ENTERED AT 10:18:46 ON 17 JAN 2007
STRUCTURE UPLOADED
D QUE STAT

L32 19 SEA SSS SAM L31 (150 REACTIONS)
D QUE STAT
D QUE

L33 366 SEA SSS FUL L31 (2195 REACTIONS)
SAVE TEMP L33 LOE105CRXP/A

FILE 'STNGUIDE' ENTERED AT 10:21:27 ON 17 JAN 2007
D QUE L7

FILE 'STNGUIDE' ENTERED AT 10:29:28 ON 17 JAN 2007

L34 FILE 'CASREACT' ENTERED AT 10:32:44 ON 17 JAN 2007
STRUCTURE UPLOADED
D QUE STAT

L35 1 SEA SUB=L33 SSS SAM L34 (1 REACTIONS)
D QUE STAT

L36 61 SEA SUB=L33 SSS FUL L34 (273 REACTIONS)
SAVE TEMP L36 LOE105CRXREF/A

FILE 'STNGUIDE' ENTERED AT 10:36:00 ON 17 JAN 2007

FILE 'HCAPLUS' ENTERED AT 10:36:37 ON 17 JAN 2007
D SCAN TI HIT L25

L37 2 SEA ABB=ON PLU=ON L25 NOT L1
D SCAN TI HIT

FILE 'STNGUIDE' ENTERED AT 10:37:11 ON 17 JAN 2007
D COST

L38 FILE 'CHEMINFORMRX' ENTERED AT 10:38:59 ON 17 JAN 2007
0 SEA SSS SAM L34 (0 REACTIONS)

FILE 'STNGUIDE' ENTERED AT 10:39:41 ON 17 JAN 2007

FILE 'CHEMINFORMRX' ENTERED AT 10:42:24 ON 17 JAN 2007
D QUE

L39 18 SEA SSS FUL L34 (58 REACTIONS)
SAVE TEMP L39 LOE105CHMP/A

FILE 'STNGUIDE' ENTERED AT 10:43:14 ON 17 JAN 2007

L40 FILE 'ZCAPLUS' ENTERED AT 10:44:45 ON 17 JAN 2007
QUE ABB=ON PLU=ON HEINELT, U?/AU

L41 QUE ABB=ON PLU=ON LANG, H?/AU

L42 QUE ABB=ON PLU=ON (AVENTIS OR SANOFI)/PA,SO,CS
FILE 'STNGUIDE' ENTERED AT 10:47:47 ON 17 JAN 2007
FILE 'HCAPLUS' ENTERED AT 10:48:13 ON 17 JAN 2007
L43 16 SEA ABB=ON PLU=ON L10 AND (L40 OR L41)
FILE 'REGISTRY' ENTERED AT 10:48:42 ON 17 JAN 2007
L44 84 SEA ABB=ON PLU=ON L6 AND (MEDLINE OR EMBASE OR BIOSIS)/LC
FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 10:49:42 ON 17 JAN 2007
L45 5270 SEA ABB=ON PLU=ON L44
L46 1 SEA ABB=ON PLU=ON L45 AND (L40 OR L41)
D SCAN
D TRI
FILE 'STNGUIDE' ENTERED AT 10:50:29 ON 17 JAN 2007
D QUE STAT L6
D QUE STAT L25
D QUE STAT L33
D QUE STAT L36
D QUE STAT L39
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:01:02 ON 17 JAN 2007
L47 82 DUP REM L25 L36 L39 (0 DUPLICATES REMOVED)
ANSWERS '1-3' FROM FILE HCAPLUS
ANSWERS '4-64' FROM FILE CASREACT
ANSWERS '65-82' FROM FILE CHEMINFORMRX
FILE 'STNGUIDE' ENTERED AT 11:02:46 ON 17 JAN 2007
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:04:53 ON 17 JAN 2007
D IBIB ED AB HITSTR
FILE 'STNGUIDE' ENTERED AT 11:04:55 ON 17 JAN 2007
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:05:11 ON 17 JAN 2007
D IBIB ED AB HITSTR 2-3
FILE 'STNGUIDE' ENTERED AT 11:05:15 ON 17 JAN 2007
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:05:53 ON 17 JAN 2007
FILE 'STNGUIDE' ENTERED AT 11:06:02 ON 17 JAN 2007
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:06:08 ON 17 JAN 2007
D IBIB ED AB FHIT 4
FILE 'STNGUIDE' ENTERED AT 11:06:20 ON 17 JAN 2007
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:07:10 ON 17 JAN 2007
D IBIB AB FHIT 5-64
FILE 'STNGUIDE' ENTERED AT 11:08:21 ON 17 JAN 2007
FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:08:47 ON 17 JAN 2007
D BIB AB FHIT 65

FILE 'STNGUIDE' ENTERED AT 11:08:50 ON 17 JAN 2007

FILE 'HCAPLUS, CASREACT, CHEMINFORMRX' ENTERED AT 11:09:03 ON 17 JAN 2007
D BIB AB FHIT 66-82

FILE 'STNGUIDE' ENTERED AT 11:09:12 ON 17 JAN 2007
D QUE NOS L43
D QUE NOS L46

L48 FILE 'HCAPLUS, MEDLINE' ENTERED AT 11:11:57 ON 17 JAN 2007
16 DUP REM L43 L46 (1 DUPLICATE REMOVED)
ANSWERS '1-16' FROM FILE HCAPLUS

FILE 'STNGUIDE' ENTERED AT 11:12:12 ON 17 JAN 2007

FILE 'HCAPLUS' ENTERED AT 11:12:31 ON 17 JAN 2007
D IBIB ED AB 1-16

FILE 'STNGUIDE' ENTERED AT 11:12:33 ON 17 JAN 2007

FILE 'STNGUIDE' ENTERED AT 11:13:55 ON 17 JAN 2007

FILE HOME

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 12, 2007 (20070112/UP).

FILE ZCAPLUS

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FILE LAST UPDATED: 16 Jan 2007 (20070116/ED)

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FILE HCAPLUS

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FILE COVERS 1907 - 17 Jan 2007 VOL 146 ISS 4
FILE LAST UPDATED: 16 Jan 2007 (20070116/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 JAN 2007 HIGHEST RN 917470-98-5
DICTIONARY FILE UPDATES: 15 JAN 2007 HIGHEST RN 917470-98-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE CASREACT

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FILE CONTENT:1840 - 14 Jan 2007 VOL 146 ISS 3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*****  
*                                                                 *  
*   CASREACT now has more than 10 million reactions             *  
*                                                                 *  
*****
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CHEMINFORMRX

FILE LAST UPDATED: 5 DEC 2006 <20061205/UP>

>>> CAS Registry Numbers are available for
substances prior to 1995 <<<

FILE MEDLINE

FILE LAST UPDATED: 16 Jan 2007 (20070116/UP). FILE COVERS 1950 TO DATE.

All regular MEDLINE updates from November 15 to December 16 have been added to MEDLINE, along with 2007 Medical Subject Headings (MeSH(R)) and 2007 tree numbers.

The annual reload will be available in early 2007.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BIOSIS

FILE COVERS 1969 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 10 January 2007 (20070110/ED)

FILE EMBASE

FILE COVERS 1974 TO 16 Jan 2007 (20070116/ED)

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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